

FIG. 1

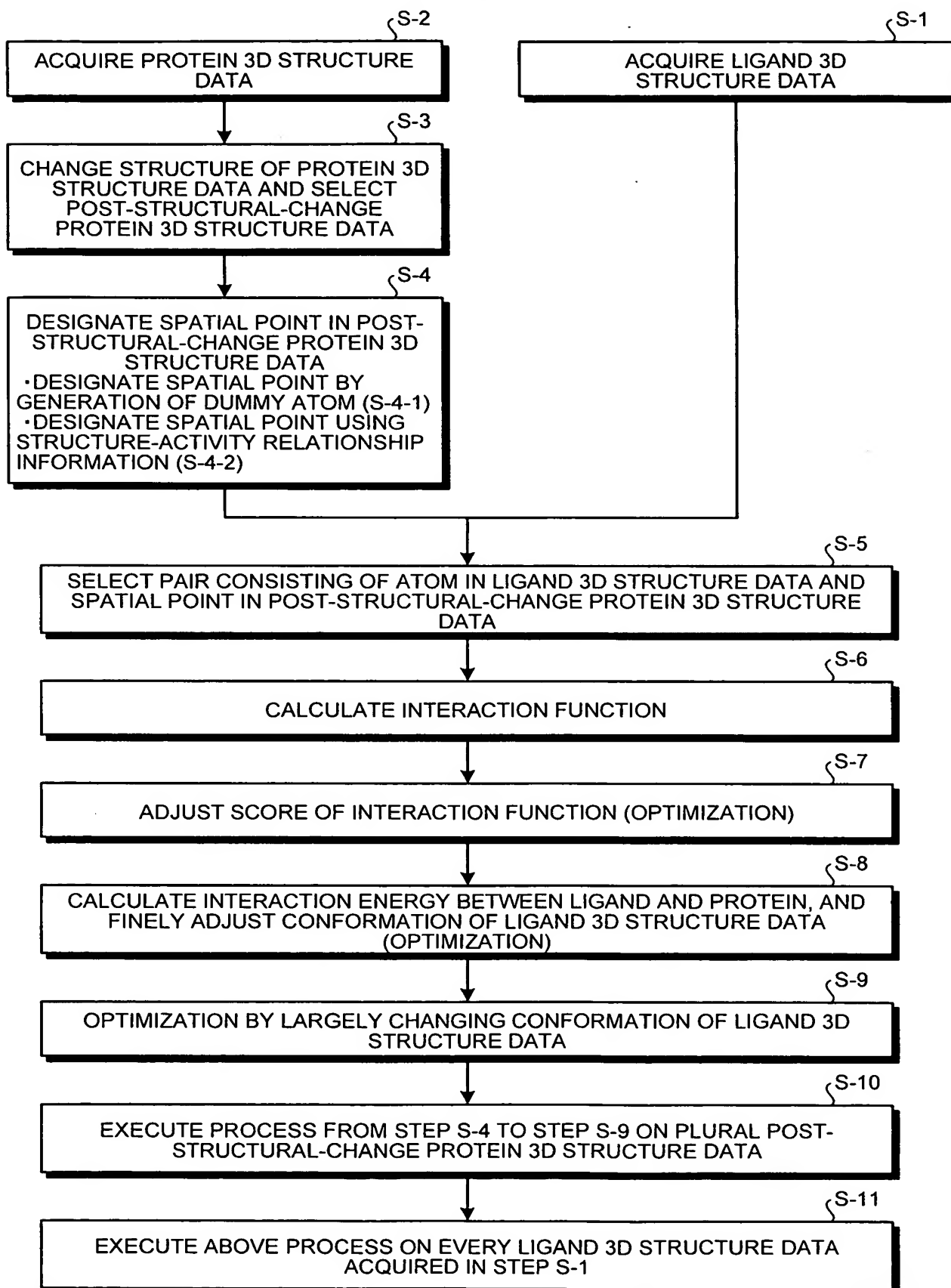


FIG.2

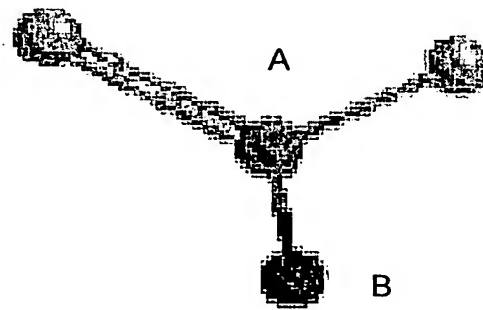


FIG.3

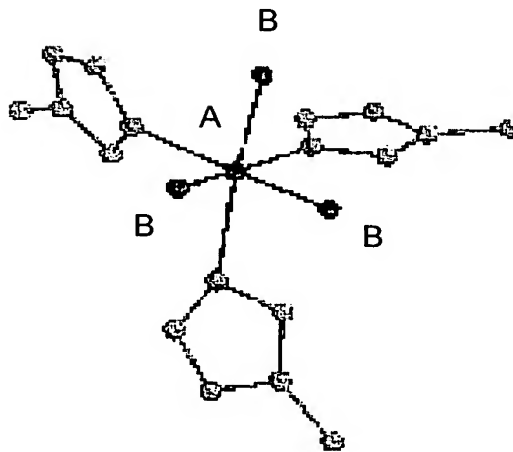


FIG.4



FIG.5

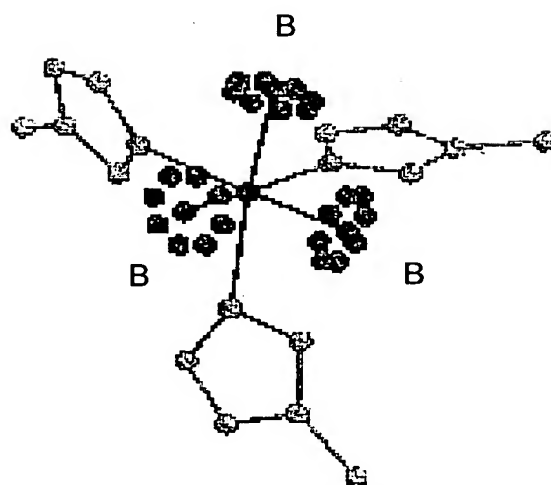


FIG.6

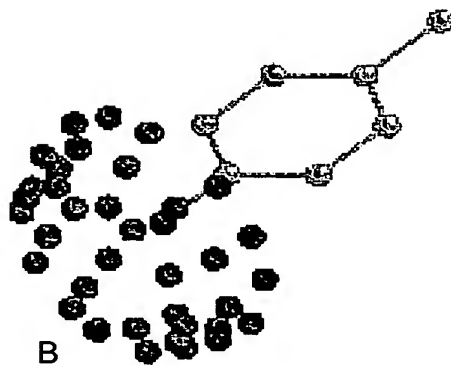


FIG.7

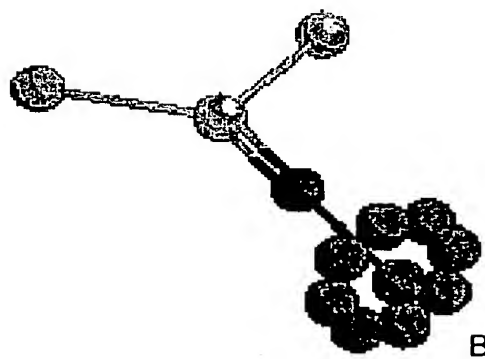


FIG.8

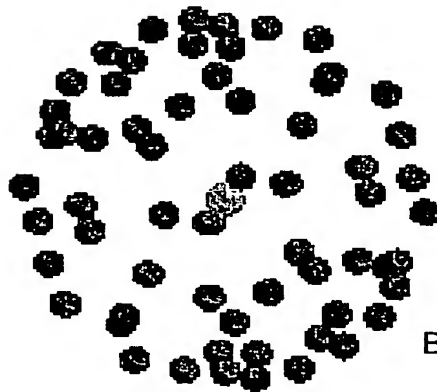


FIG.9

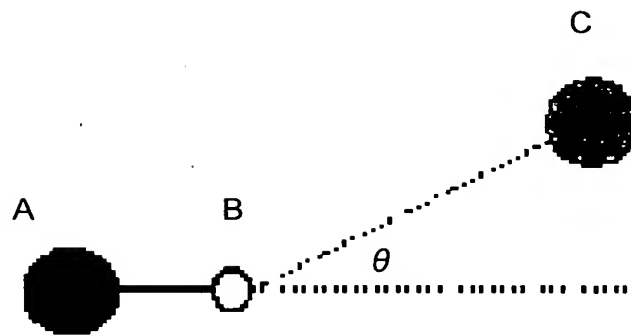


FIG.10

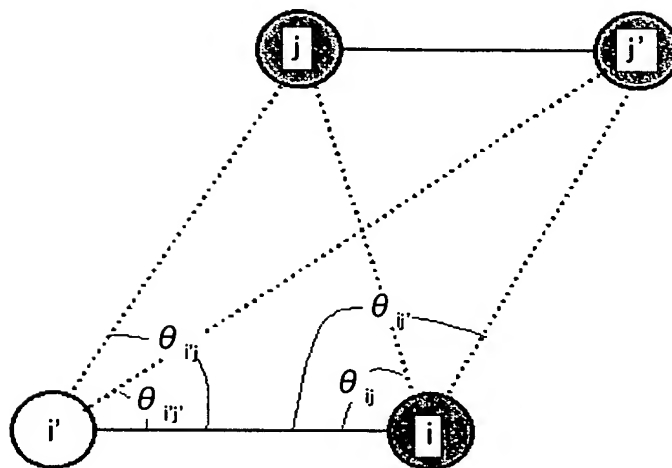


FIG.11

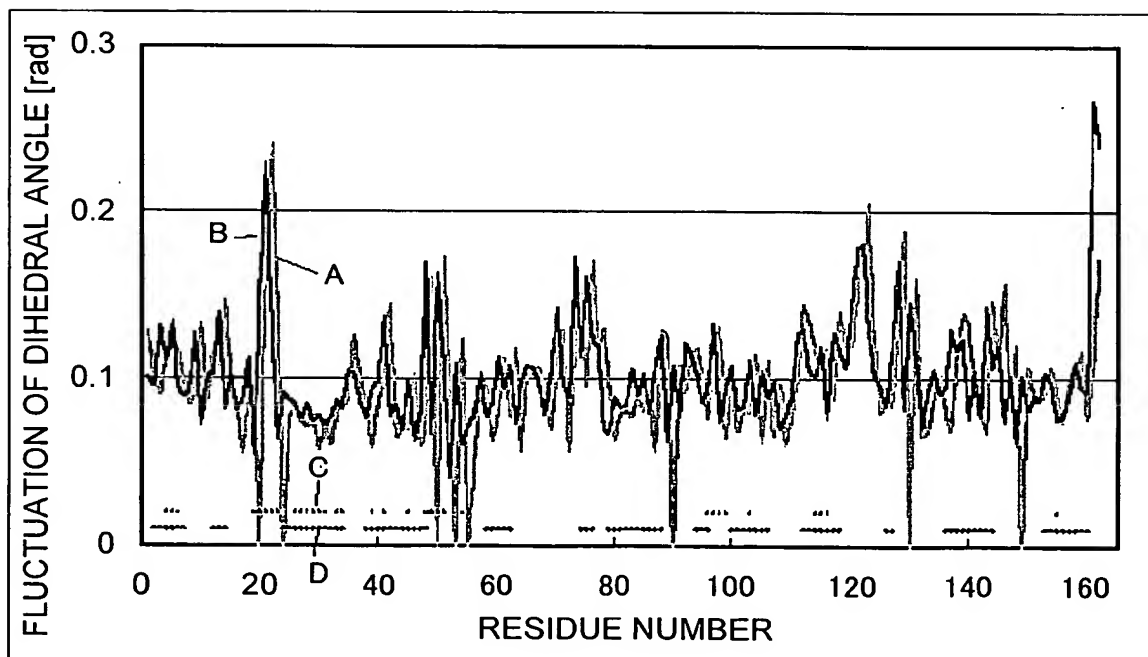


FIG.12

RANKING	MINIMUM VALUE	MAXIMUM VALUE	$\alpha$ [%]	$\beta$ [Å]	NUMBER OF CLUSTERS	SCORE
1	0	800	70	0.4	57	0.9054
2	0	800	70	0.1	62	0.9097
3	0	800	70	0.2	62	0.9097
4	0	800	70	0.3	62	0.9097
5	0	800	80	0.1	81	0.9102
6	0	800	80	0.2	81	0.9102
7	0	800	70	0.5	52	0.9103
8	0	800	80	0.4	73	0.9106
9	0	800	80	0.3	80	0.9116
10	0	800	80	0.5	67	0.9151
11	0	800	70	0.6	46	0.9156
12	0	800	90	0.5	240	0.9183
13	0	800	90	0.6	174	0.9194
14	0	800	60	0.6	13	0.9211
15	0	800	90	0.4	297	0.9225
16	0	800	80	0.6	58	0.9261
17	0	800	90	0.1	425	0.9286
18	0	800	90	0.2	425	0.9286
19	0	800	90	0.3	420	0.9296
20	0	800	60	0.1	16	0.9354
21	0	800	60	0.2	16	0.9354
22	0	800	60	0.3	16	0.9354
23	0	800	60	0.4	16	0.9354
24	0	800	60	0.5	15	0.9451
25	600	900	60	0.1	28	0.9469
26	600	900	60	0.2	28	0.9469
27	600	900	60	0.3	28	0.9469
28	600	900	60	0.4	28	0.9469
29	600	900	60	0.5	27	0.9518
30	600	900	60	0.6	27	0.9518

FIG.13

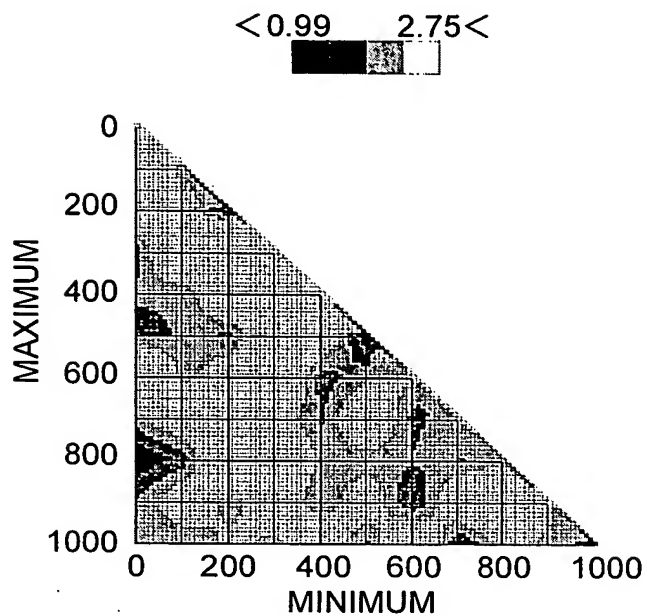


FIG.14

MINIMUM VALUE OF CONSTRAINED MD	0.00
MAXIMUM VALUE OF CONSTRAINED MD	800.00
CLUSTERING COEFFICIENT $\alpha$ (%)	80.00
CLUSTERING COEFFICIENT $\beta$ (Å)	0.40



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FIG.15

<0.94 2.70<

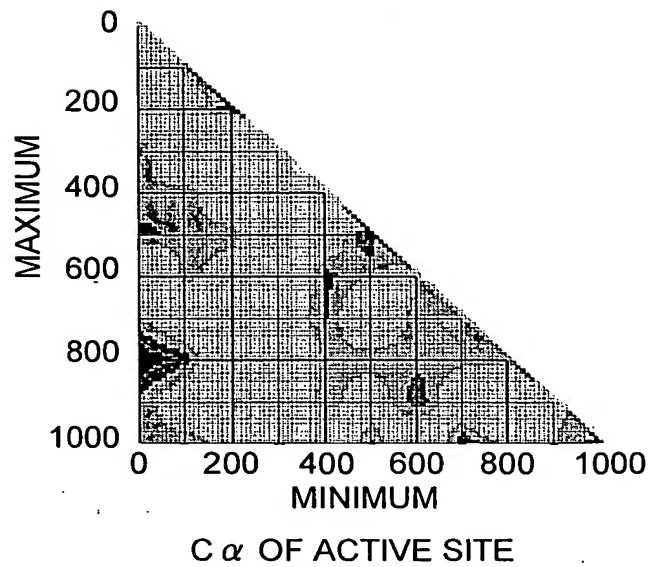
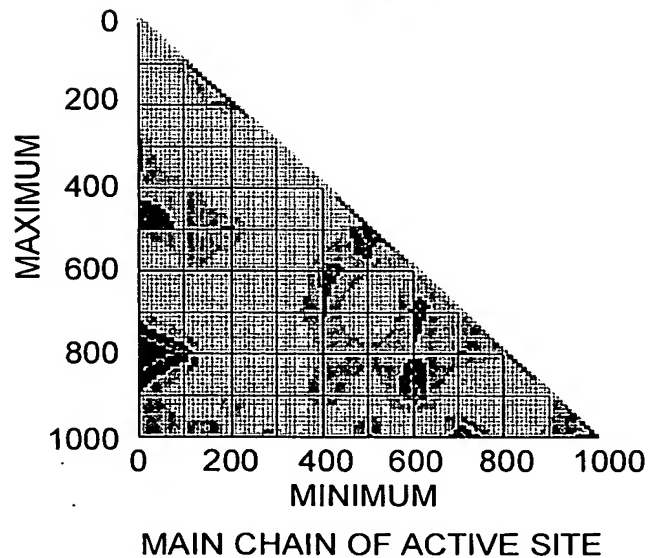


FIG.16

<0.99 2.75<



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FIG.17

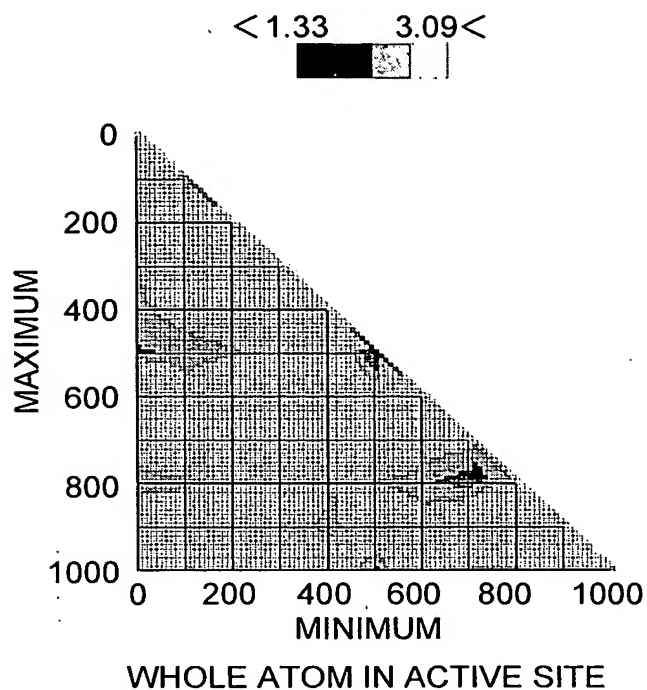


FIG.18

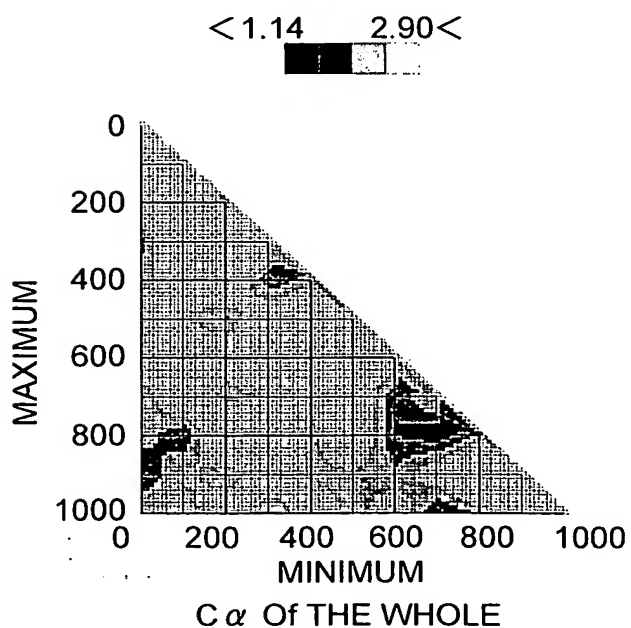


FIG.19

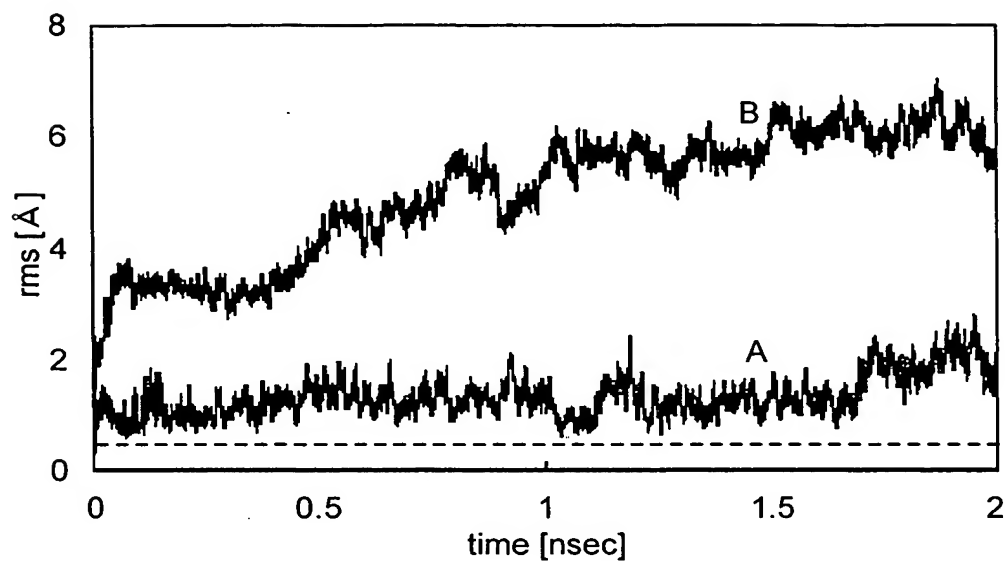
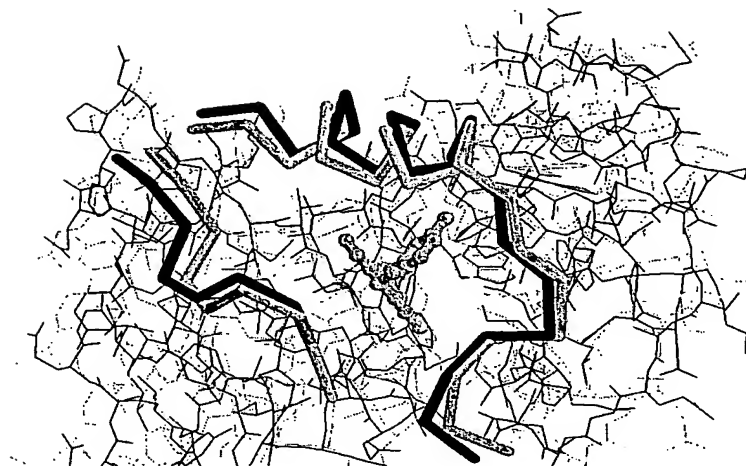


FIG.20



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FIG.21



## FIG.22

>1CBQ  
PNFSGNWKIIRSENFEELLKVLGVNVMRLRKIAVAAASKPAVEIKQEGDTFYIKTSTTVRTTEINFKVGEFFEEQTVDGRP  
CKSLVKWESENKMVCEQKLLKGEPKTSWTRELTNDGELILMTADDVCTRYYVRE  
>1CM  
-AFDGTWKVDRNENYEKFMKMGINVVKRKLGAHDNLKLITQEGNKFTVKESNFRNIDVVFELGVDFAYSLADGTE  
L-TGTWTMEGNKLVGKFRV-DNGKELIAVREIS-GNELIQTYTYEGVEAKRIFKKE

FIG.23

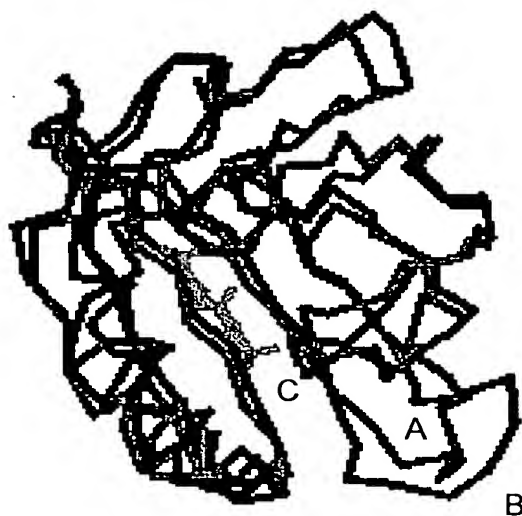
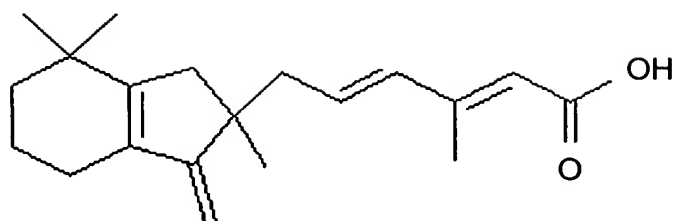


FIG.24



## FIG.25

X-RAY STRUCTURE	1CBQ
REFERENCE PROTEIN	1ICM
HOMOLOGY [%]	32.1
NUMBER OF RESIDUES	136
MAIN CHAIN IN ACTIVE SITE [Å]	2.2487
SIDE CHAIN IN ACTIVE SITE [Å]	3.2446
ALL ATOMS IN ACTIVE SITE [Å]	2.7728
MAIN CHAIN IN THE WHOLE [Å]	2.2075
SIDE CHAIN IN THE WHOLE [Å]	3.7881
ALL ATOMS IN THE WHOLE [Å]	3.0959

FIG.26

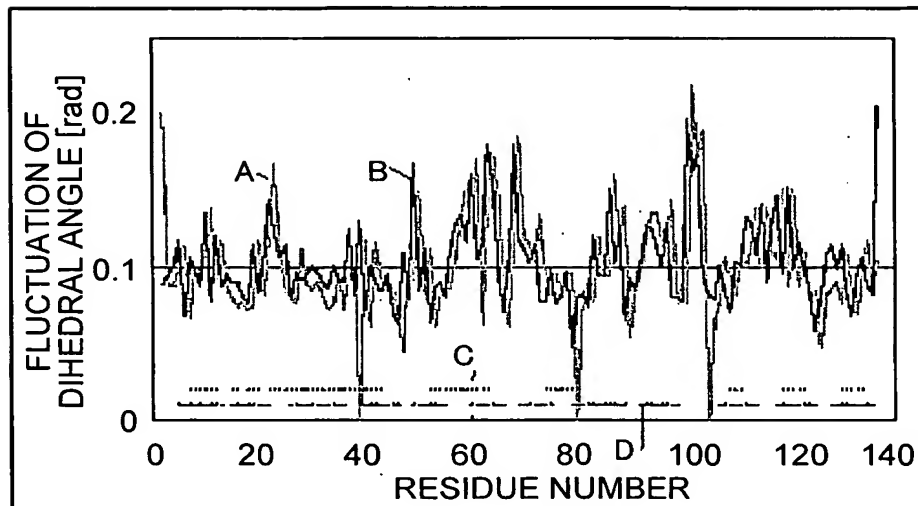


FIG.27

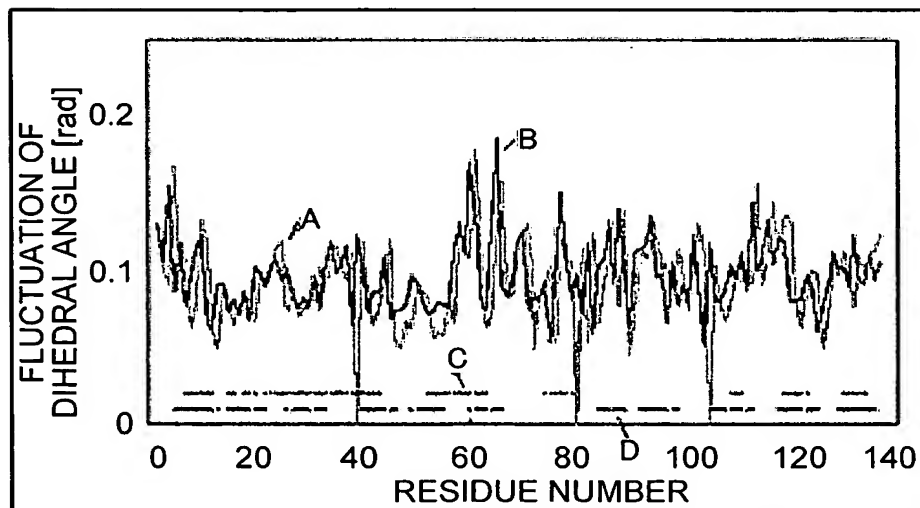
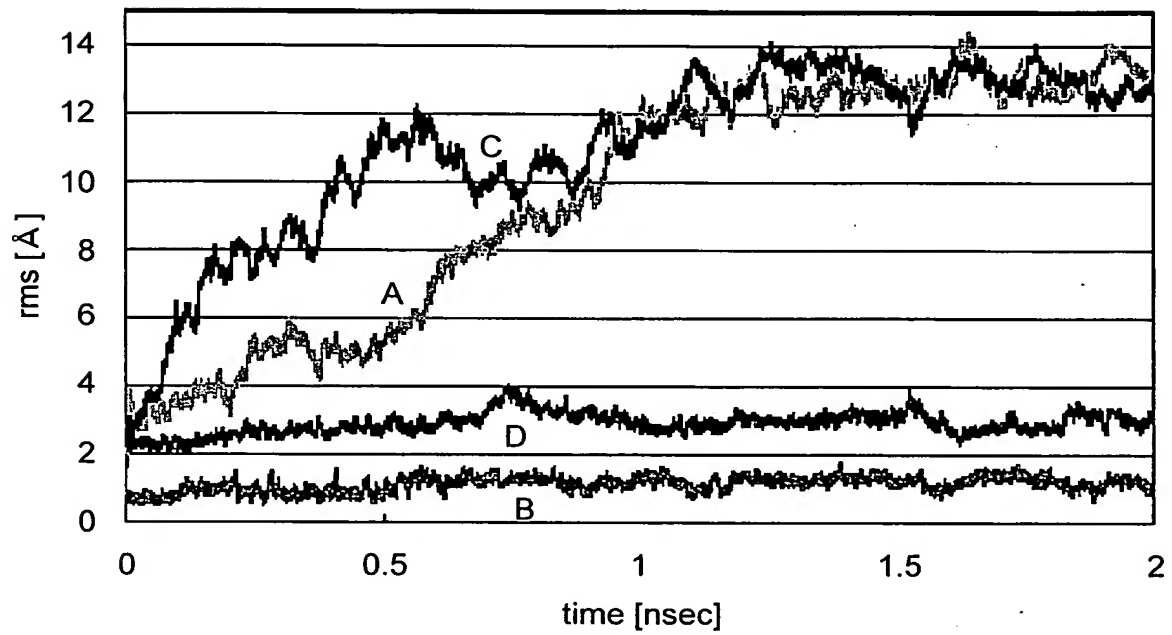




FIG.28



## FIG.29

```
>1J9G
AKALIVYGSTTGNTTEYTAETIARELADAGYEVDSDRDAASVEAGGLFEGFDLVLLGCSTWGD-DCIELQDDDFIPLFDSLEE
TGAQGRKVAACFGCGDS--SYEYFCGAVDAIEEKLKNLGAENVQDG-----LRIDGDPRAARDI
VGWAHHDVRGAI
>1AHN
AITGIFFGSDTGNTENIAKMIQKQLGKDVADVHDIAKSSKE---DLEAYDILLGIPTWYGY---EAQCDWDDFFPTLEE
IDFNGKLVALFGCGDQEDYAEYFCDALGTIRDIIEPRGATIVGHWPTAGYHFEASKGLADDDHFFVGLAIDEDRQPETA
RVEKWKQISE
```

FIG.30

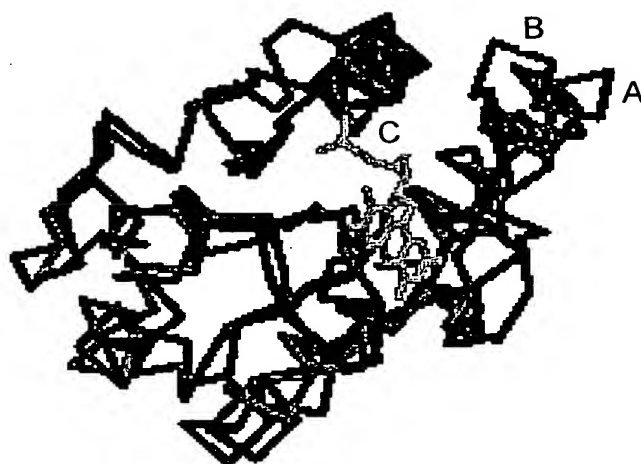
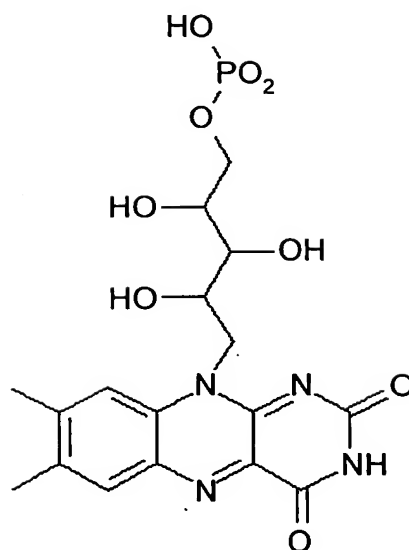


FIG.31



## FIG.32

X-RAY STRUCTURE	1J9G
REFERENCE PROTEIN	1AHN
HOMOLOGY [%]	29.2
NUMBER OF RESIDUES	147
MAIN CHAIN IN ACTIVE SITE [Å]	2.3909
SIDE CHAIN IN ACTIVE SITE [Å]	4.5774
ALL ATOMS IN ACTIVE SITE [Å]	3.5753
MAIN CHAIN IN THE WHOLE [Å]	3.1212
SIDE CHAIN IN THE WHOLE [Å]	5.367
ALL ATOMS IN THE WHOLE [Å]	4.315

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FIG.33

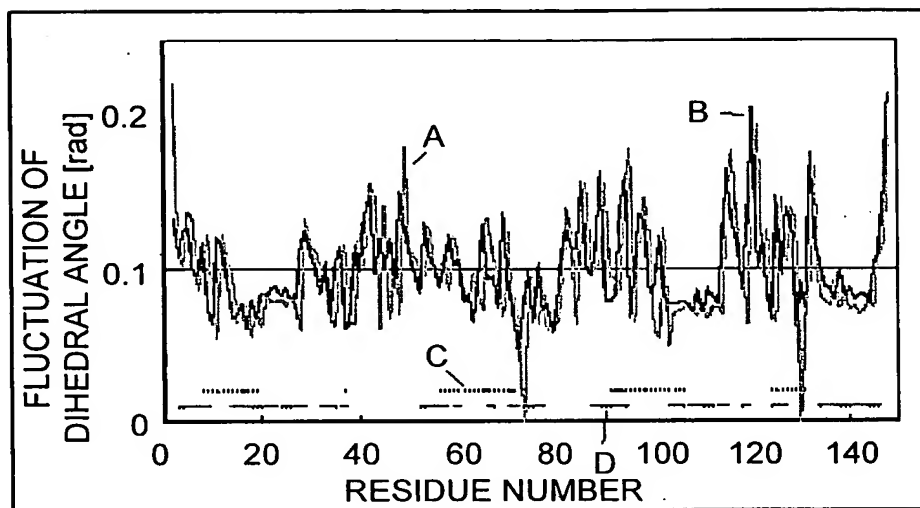


FIG.34

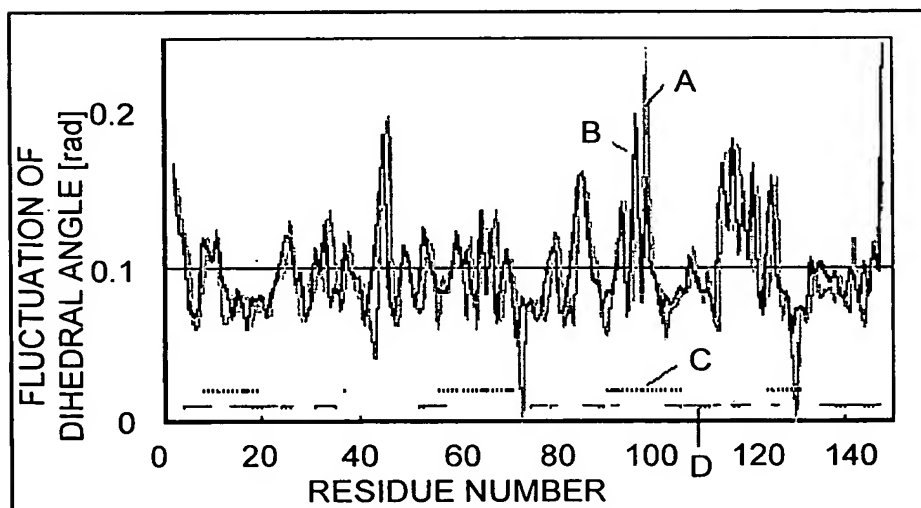
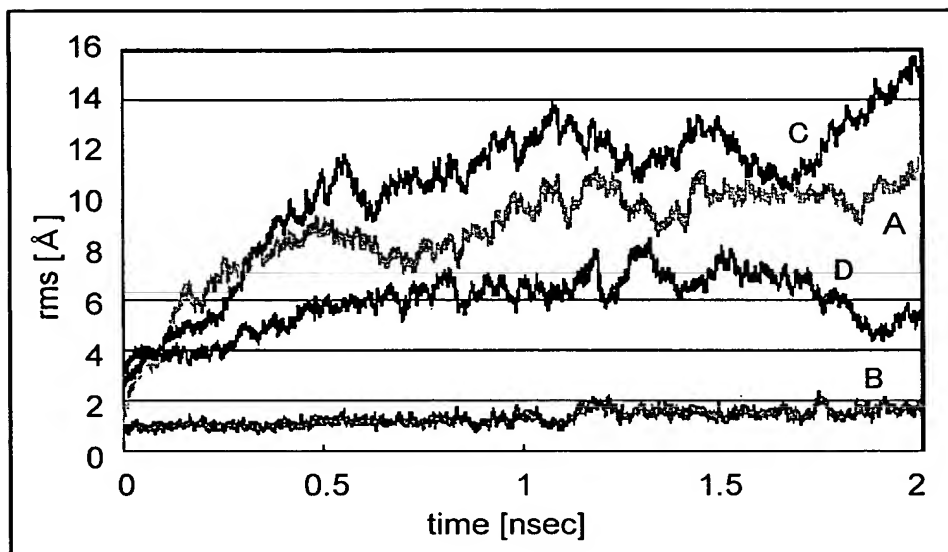


FIG.35



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## FIG.36

>1MMB  
NPKWERTNLT YRIRNYTPQLSEAEVERAIKDAFELWSVASPLIFTRISQQGEADINIAFYQRDHGDNSPFDGPNGLAHAF  
QPGQGIGGDAHFDAEETWTNTSANYNLFLVAAHEFGHSLGLAHSSDPGALMYPNYA-FRETSNYSPLPQDDIDGIGAIYG  
>1B3D A  
IPKWRKTHLT YRIVNYTPDLPKDAVDSAVEKALKVWEEVTPLTFSRLYEGEADIMISFAVREHGDFYPFDGPGNVLAHAY  
APGPGINGDAHFDDDEQWTKD TTGTNLFVAAHEIGHSLGLFHSANTEALMYPLYHSLTDLTRFRLSQDDINGIQSLYG

FIG.37

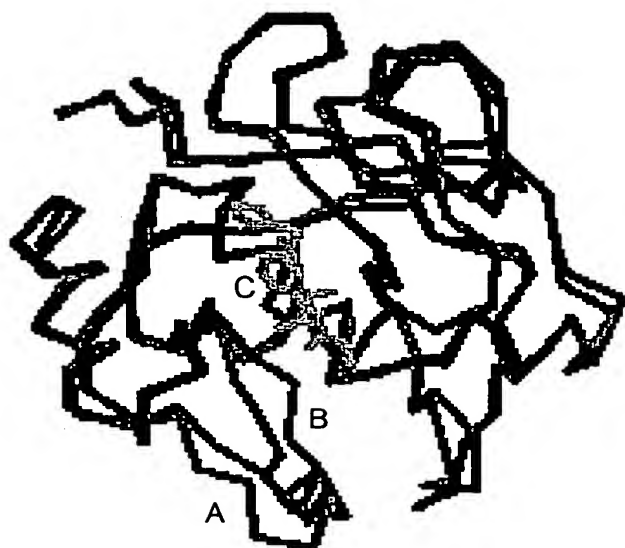
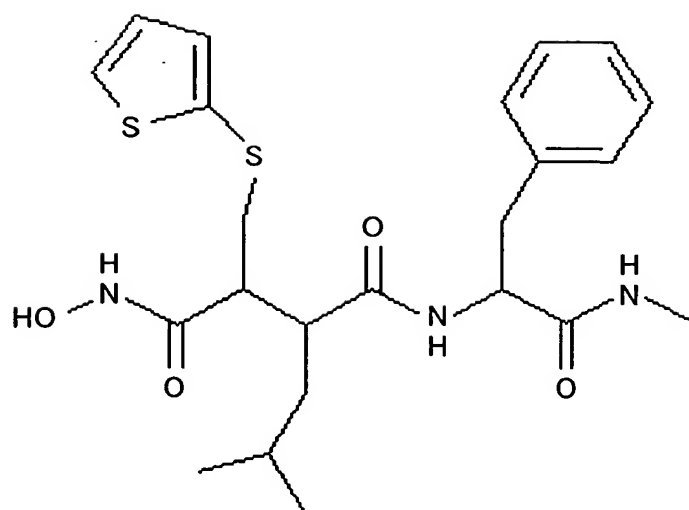


FIG.38





## FIG.39

X-RAY STRUCTURE	1MMB
REFERENCE PROTEIN	1B3D
HOMOLOGY [%]	55
NUMBER OF RESIDUES	158
MAIN CHAIN IN ACTIVE SITE [Å]	0.9442
SIDE CHAIN IN ACTIVE SITE [Å]	3.0756
ALL ATOMS IN ACTIVE SITE [Å]	2.2417
MAIN CHAIN IN THE WHOLE [Å]	1.1339
SIDE CHAIN IN THE WHOLE [Å]	2.5715
ALL ATOMS IN THE WHOLE [Å]	1.9808

FIG.40

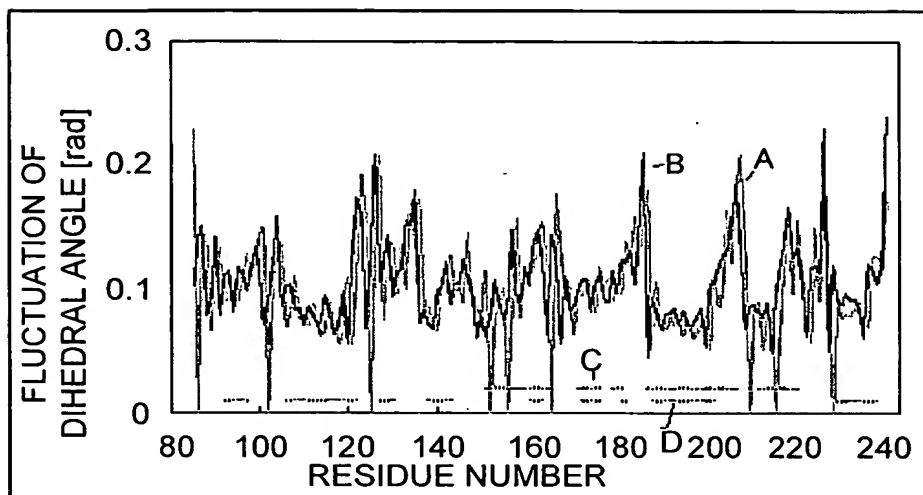


FIG.41

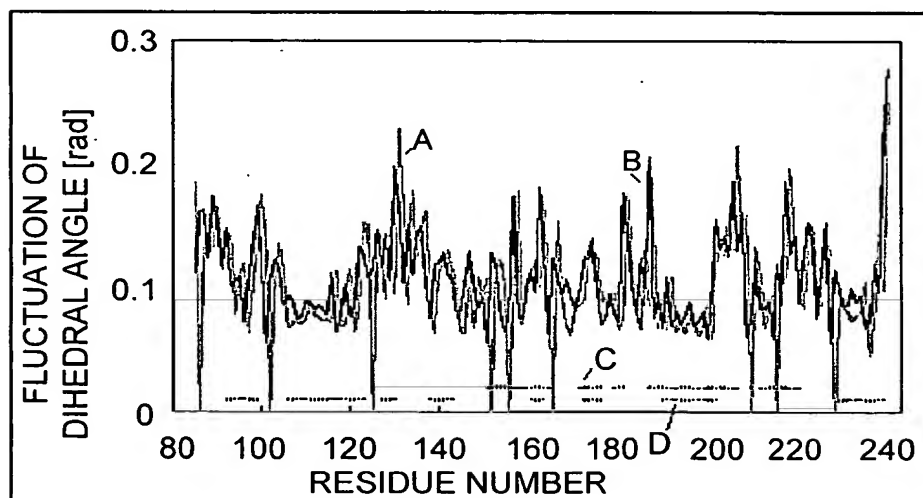


FIG.42

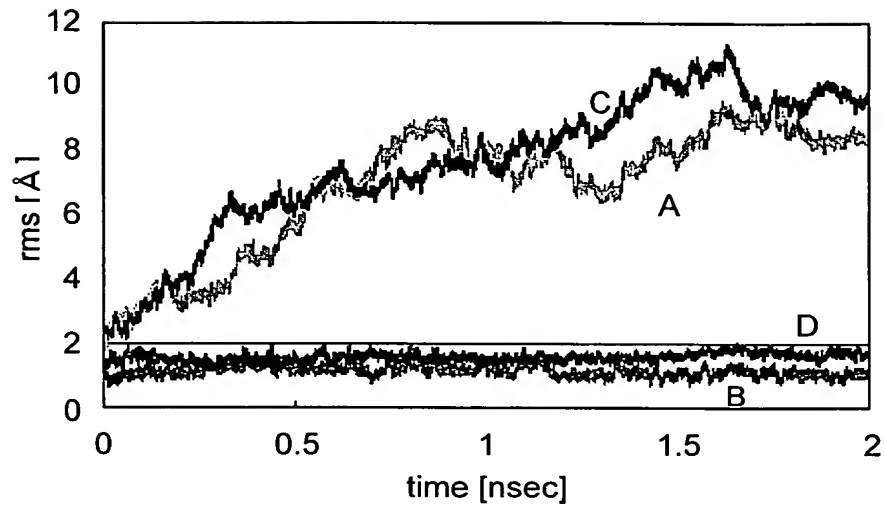


FIG.43

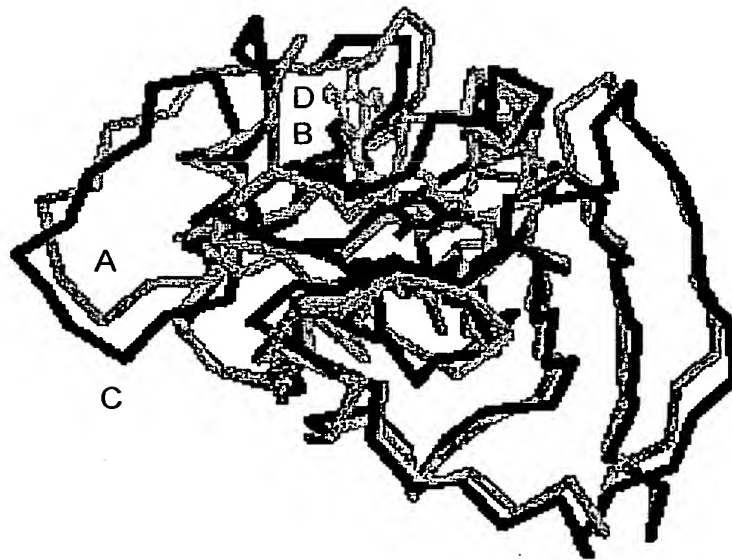


FIG.44

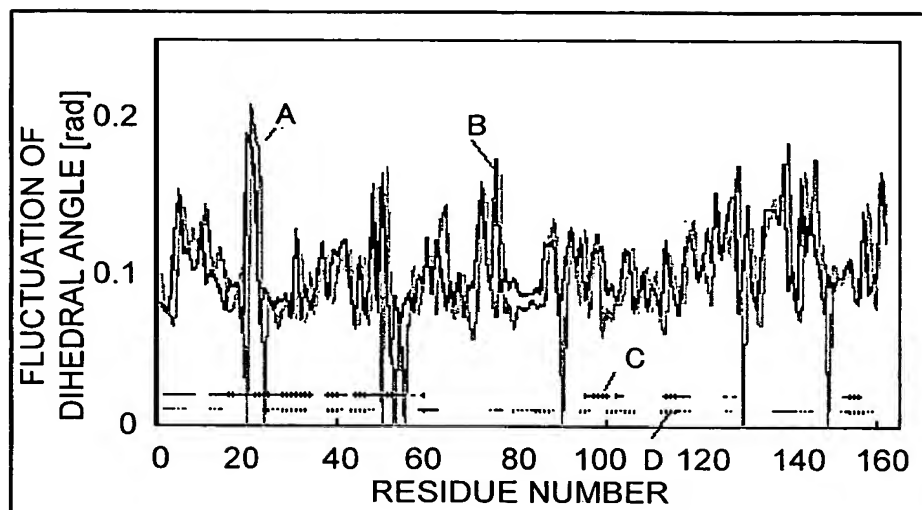


FIG.45

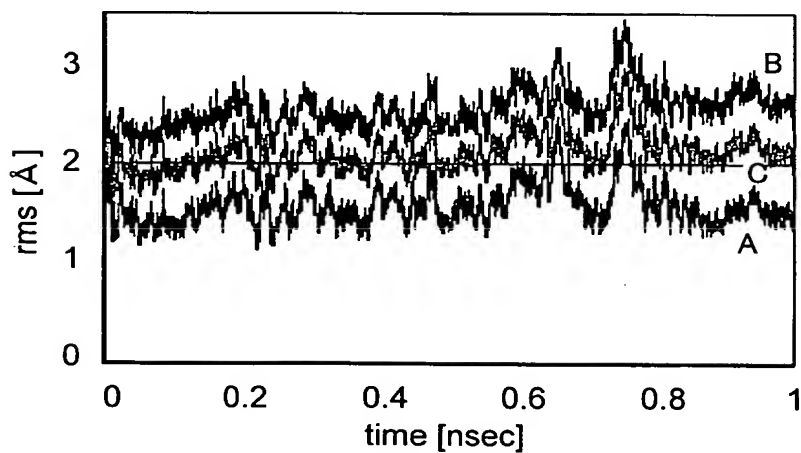


FIG.46

ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
LUE4 O	N.pl3	300	2.87
ASP26 OD1	N.ar	300	3.00
ASP26 OD2	N.pl3	300	3.00

FIG.47

SECTION [nsec]	DISTANCE [fsec]	NUMBER OF CLUSTERS	MAIN CHAIN [Å]	ALL ATOMS [Å]	LIGAND [Å]
INITIAL STRUCTURE			1.5313	1.9190	
0~0.1	100	11	1.3531	1.8612	1.2734
0~1.0	100	204	1.2522	1.8116	0.9614
0~1.0	1000	26	1.2522	1.8116	0.8169

FIG.48

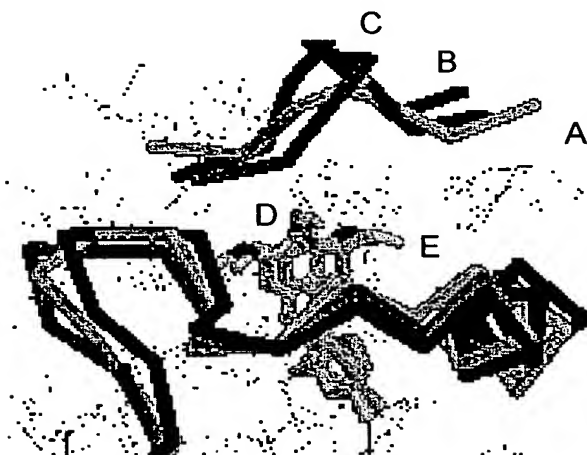


FIG.49

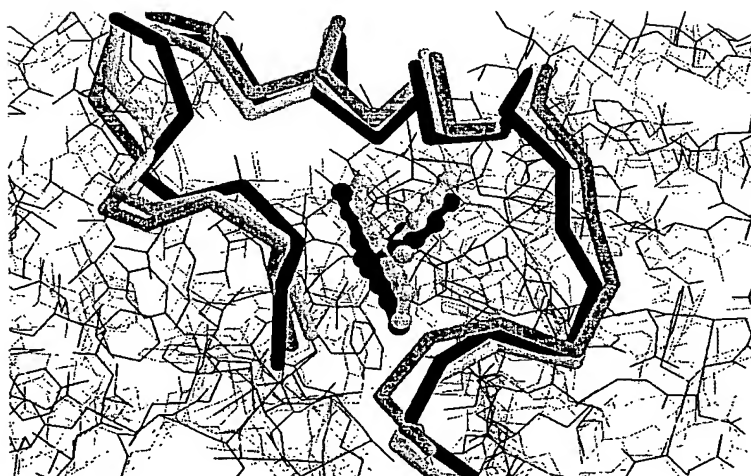


FIG.50

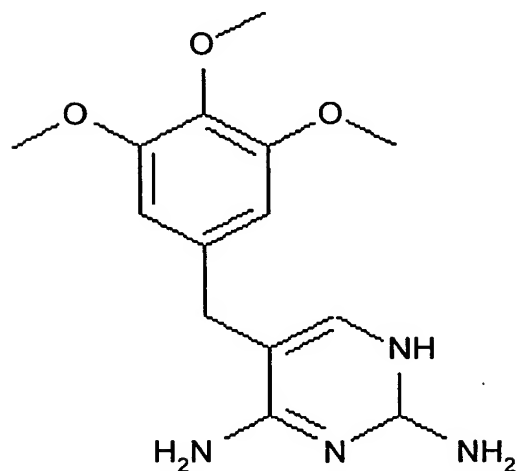


FIG.51

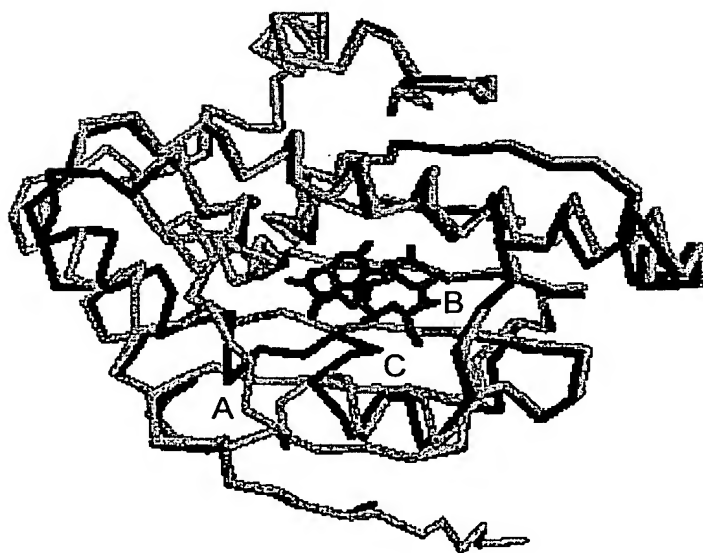


FIG.52

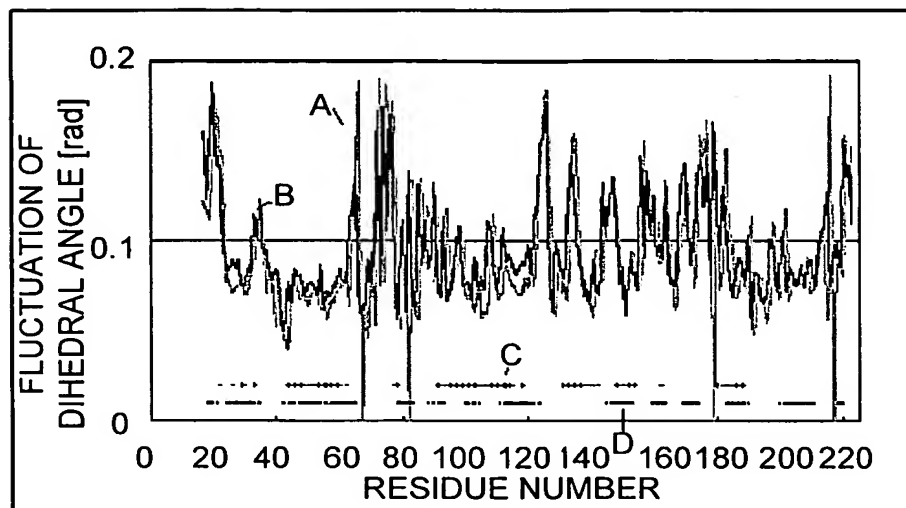


FIG.53

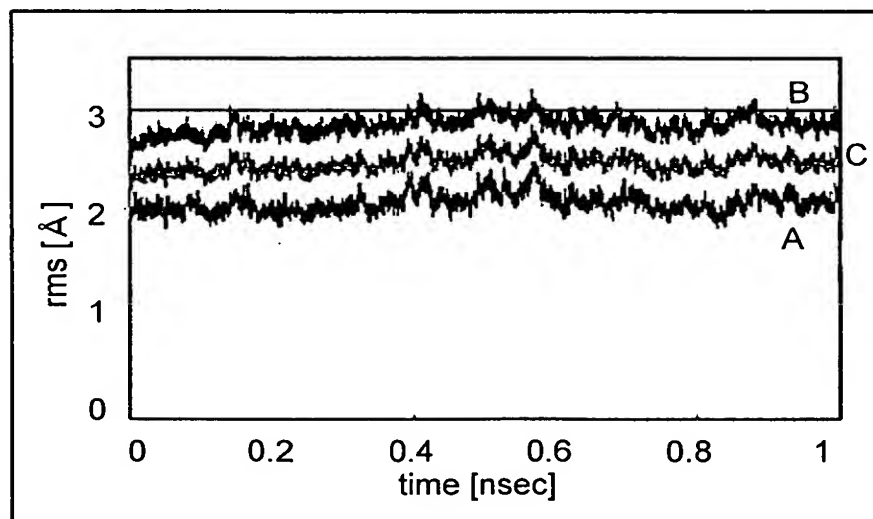




FIG.54

ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
LYS58 NZ	O.3	300	2.8
ASP93 OD2	N.am	300	2.8
PHE138 N	O.2	300	2.8

FIG.55

SECTION [nsec]	DISTANCE [fsec]	NUMBER OF CLUSTERS	MAIN CHAIN [Å]	ALL ATOMS [Å]	LIGAND [Å]
INITIAL STRUCTURE			2.0144	2.2600	
0~0.1	100	6	1.8525	2.2601	1.2081
0~1.0	100	133	1.9139	2.3883	1.5932
0~1.0	1000	9	1.9764	2.8421	0.9667

FIG.56

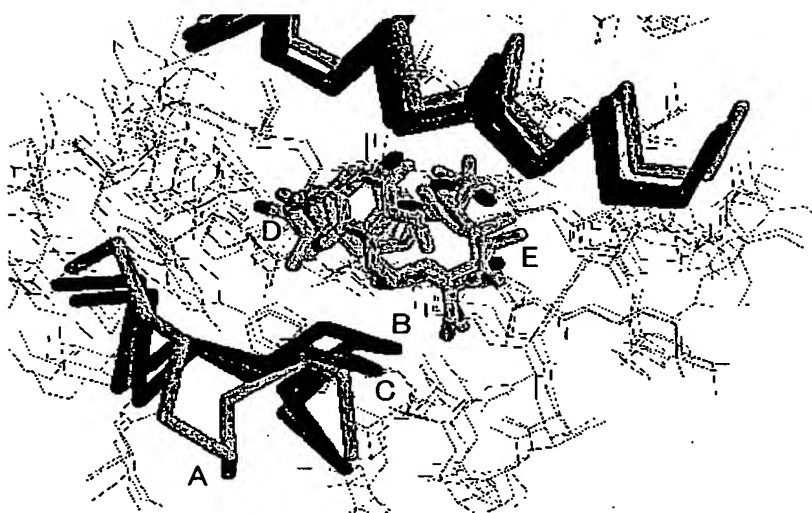


FIG.57

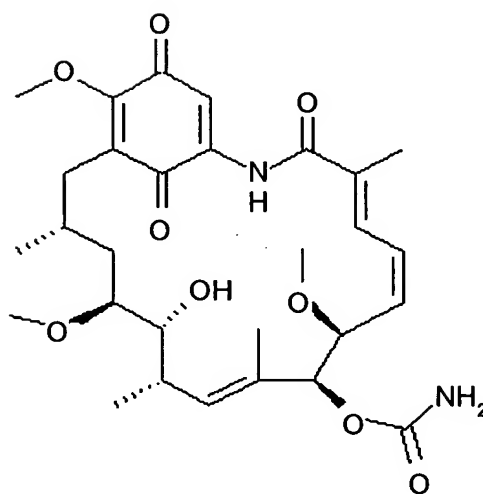


FIG.58



FIG.59

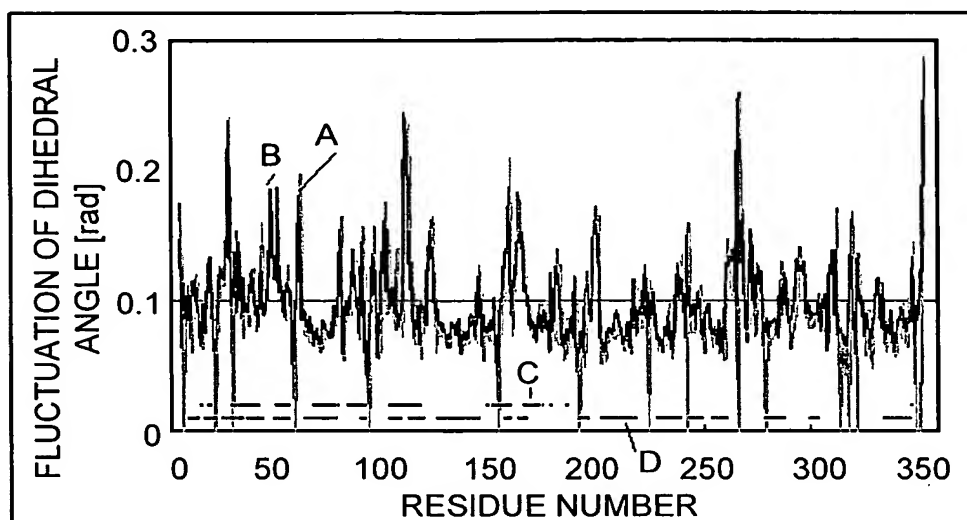
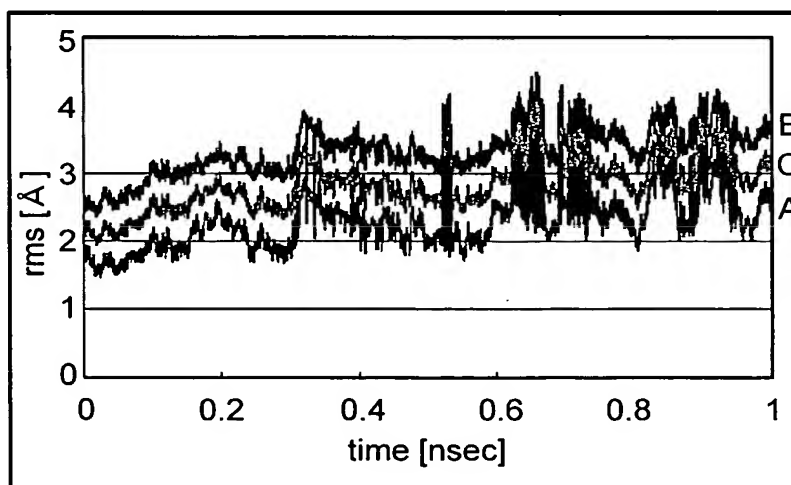


FIG.60



## FIG.61

ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
LEU75 CD1	F	300	3.6
LEU75 CD2	F	300	3.6
MET109 N	N.ar	300	2.7

## FIG.62

SECTION [nsec]	DISTANCE [fsec]	NUMBER OF CLUSTERS	MAIN CHAIN [Å]	ALL ATOMS [Å]	LIGAND [Å]
INITIAL STRUCTURE			1.7972	2.1606	
0~0.1	100	5	1.6101	2.0766	1.6112
0~1.0	100	319	1.7236	2.2843	1.4550
0~1.0	1000	31	1.7236	2.2843	1.4571

FIG.63



FIG.64



FIG.65

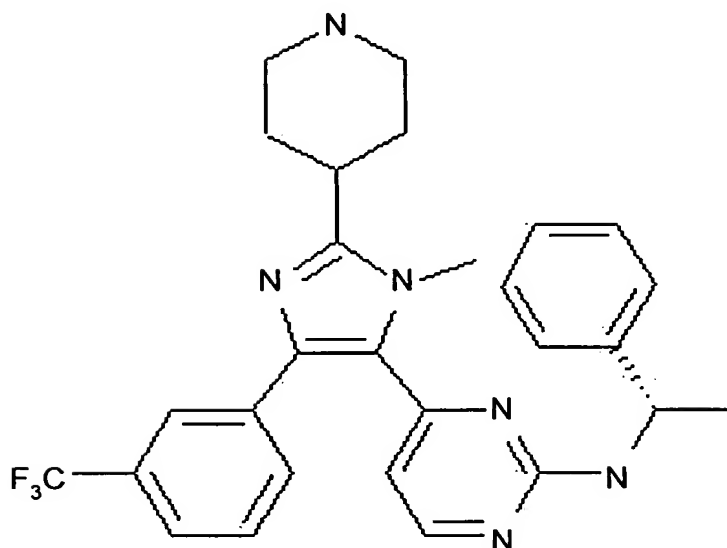


FIG.66



Title: LIGAND SEARCHING DEVICE,  
LIGAND SEARCHING METHOD,  
PROGRAM, AND RECORDING  
MEDIUM

Inventor(s): Hideaki UMEYAMA et al.  
Appl. No.: Unassigned

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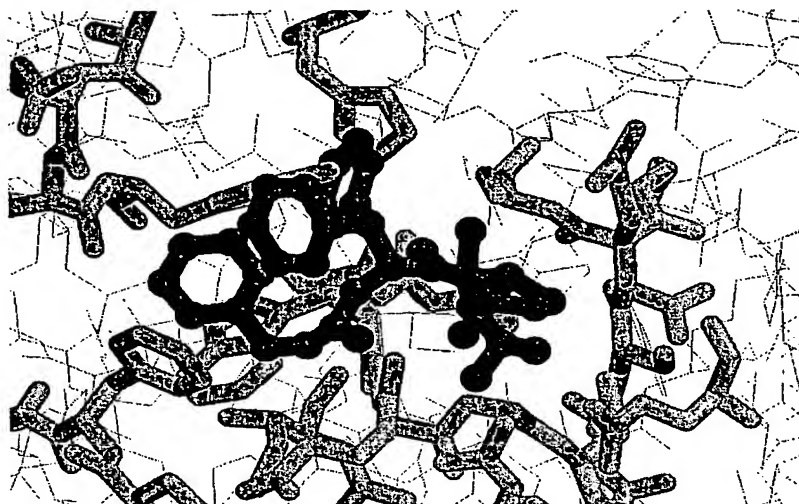
FIG.67

RANKING	INTERACTION ENERGY	PDBcode	RANKING	INTERACTION ENERGY	PDBcode
[001]	-3847.2147	4PGT	[002]	-3671.4754	1MP7
[003]	-3056.6135	1BMN	[004]	-2923.8680	1I32
[005]	-2872.4420	5FWG	[006]	-2608.5702	1LHF
[007]	-2528.6110	1BX6	[008]	-2439.5657	1B8Y
[009]	-2433.9052	1EZF	[010]	-2382.8539	5LDH
[011]	-2248.0139	1FVP	[012]	-2247.3089	1JJQ
[013]	-2133.5942	1IL2	[014]	-2128.4540	1BJI
[015]	-2125.1405	1DMT	[016]	-2103.1434	1K22
[017]	-2092.6654	1HY7	[018]	-2025.5091	966C
<b>[019]</b>	<b>-2013.9064</b>	<b>1AIX</b>	[020]	-1989.1635	1A4Q
[021]	-1946.4497	1VZE	[022]	-1932.9896	1KVO
[023]	-1928.3650	1D6V	[024]	-1901.6172	1C0A
[025]	-1890.2208	1DB5	[026]	-1867.0754	1GUH
[027]	-1855.6184	1QIN	[028]	-1817.4767	1M21
[029]	-1782.5387	1KCI	[030]	-1766.9010	1KZK
[031]	-1728.2876	6GSX	[032]	-1709.9359	2PRG
[033]	-1699.2351	1NPW	[034]	-1694.4086	2UPJ
<b>[035]</b>	<b>-1661.4315</b>	<b>1AUJ</b>	[036]	-1658.1970	1HFR
[037]	-1654.2430	1DMP	<b>[038]</b>	<b>-1599.5870</b>	<b>1F0R</b>
[039]	-1595.7907	2GSQ	[040]	-1569.9256	1QHC
[041]	-1530.3871	1AIM	[042]	-1481.1846	1EL3
[043]	-1473.7372	1QH5	[044]	-1453.3935	1LHC
[045]	-1411.1465	1HFC	[046]	-1389.8129	2FMB
[047]	-1372.1506	1GFW	[048]	-1352.8868	1EM6
[049]	-1329.5658	1AU0	[050]	-1306.5704	1M9B
[051]	-1287.3729	1EAS	[052]	-1265.8962	1LHE
[053]	-1248.8527	1C8T	[054]	-1244.2458	1MMQ
[055]	-1216.6454	1QIP	[056]	-1200.9810	207D
[057]	-1175.5120	1HWL	[058]	-1138.1881	4UPJ
[059]	-1112.7163	3GST	[060]	-1068.0641	1LEE
[061]	-1030.5972	1GA9	[062]	-1030.4960	1OD7
[063]	-1029.0345	1HOV	[064]	-1018.1686	1LF2
[065]	-1011.9100	1ODY	[066]	-976.1041	1CQQ
[067]	-948.0992	1G2K	[068]	-936.9058	2AIM
[069]	-934.4739	1NWL	[070]	-924.6255	6FIV
[071]	-902.7587	1YEI	[072]	-900.4131	1MXT
[073]	-894.5544	1YEF	[074]	-874.9274	1DZT
[075]	-857.5373	1QF0	[076]	-851.1669	1EGV
[077]	-844.2406	1F29	[078]	-824.5393	1KV2
[079]	-820.4913	456C	<b>[080]</b>	<b>-775.9659</b>	<b>1K1M</b>
[081]	-766.8359	1JR4	[082]	-763.2825	2KCE
[083]	-739.3676	1KN4	[084]	-733.8593	1RT2
[085]	-728.8765	1HPV	[086]	-718.5795	2BBQ
[087]	-705.3978	1MS6	[088]	-695.0241	1IF7
[089]	-689.7998	1JIL	[090]	-684.7289	1A8J
[091]	-676.3861	1FL3	[092]	-628.8081	1CIZ
[093]	-619.2121	1DIF	[094]	-604.7057	2BPX
[095]	-598.4143	1IF9	[096]	-564.5807	1K0C
[097]	-561.6472	1KN2	[098]	-541.1021	1HBV
[099]	-507.6808	1DB4	[100]	-496.0550	1K1J

BOLD: LIGAND CONTAINED IN 1AIX  
ITALIC: SERINE PROTEASE

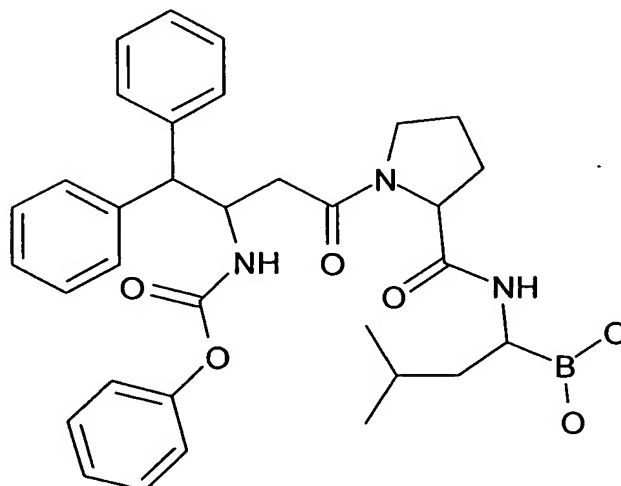


FIG.68



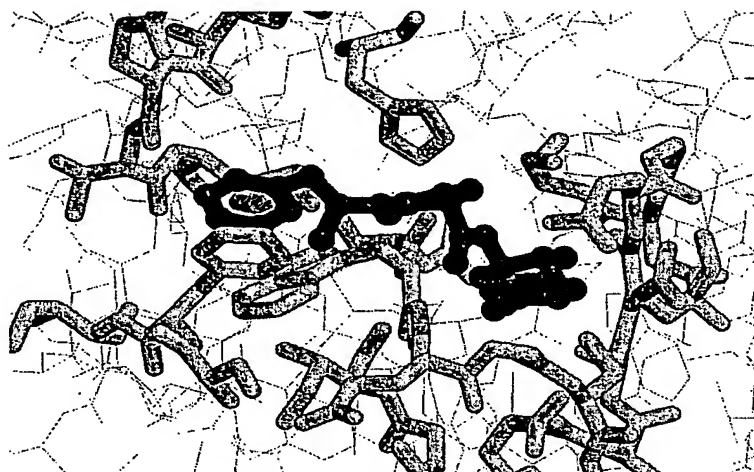
RANKING 19

FIG.69



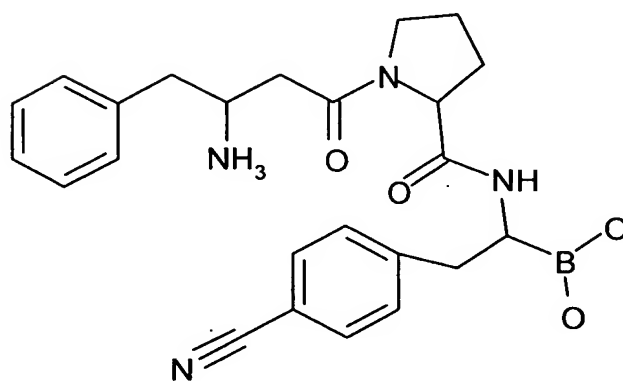
LIGAND CONTAINED IN 1AIX

FIG.70



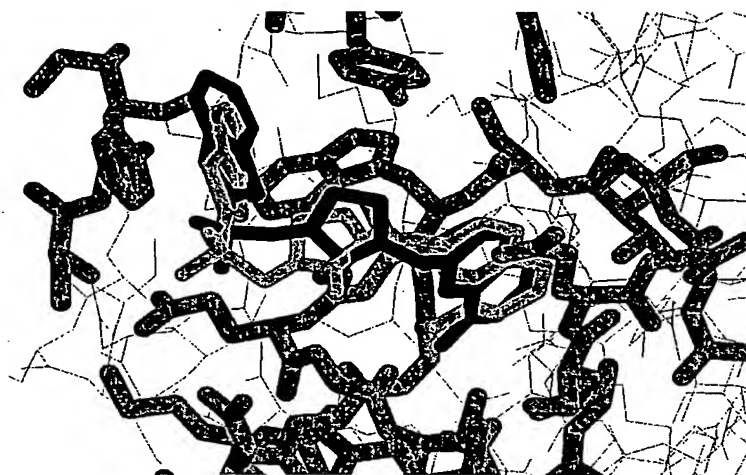
RANKING 35

FIG.71



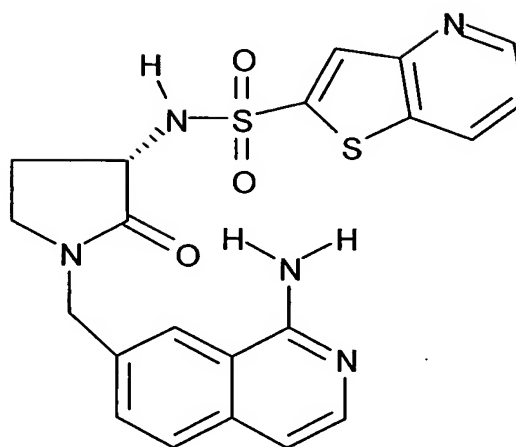
LIGAND CONTAINED IN 1AUJ

FIG.72



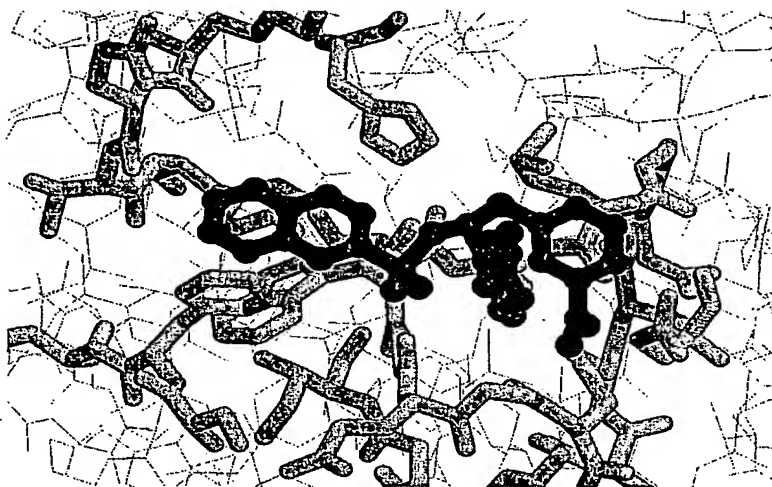
RANKING 38

FIG.73



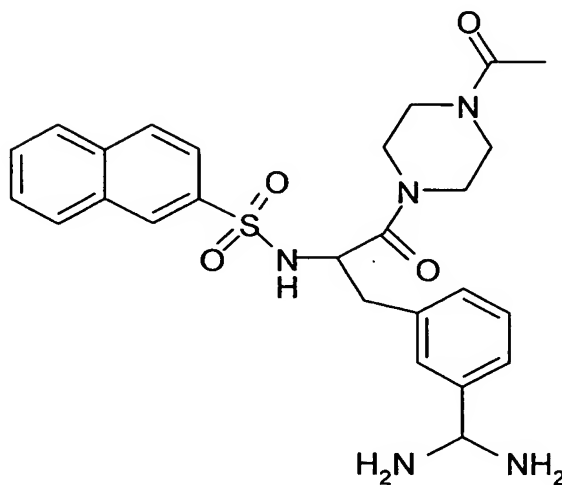
LIGAND CONTAINED IN 1FOR

FIG.74



RANKING 80

FIG.75



LIGAND CONTAINED IN 1KIM

FIG.76



FIG.77

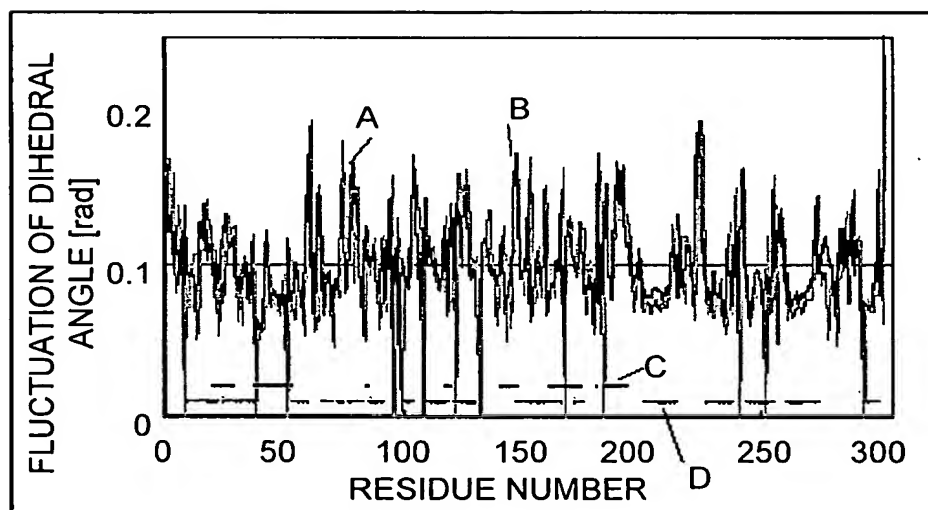


FIG.78

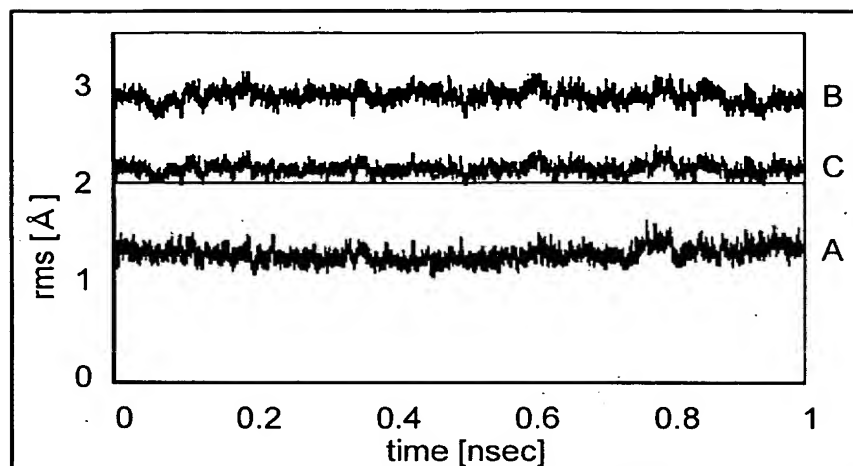


FIG.79

ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
CYS145 N	O.co2	100	2.70
MET165 CG	C.3	100	4.00
GLU166 N	O.2	100	2.70
THR190 N	O.3	100	2.70

FIG.80

RANKING	ENERGY	PDB code	REMARKS
1	-1089.2153	1QF4	ligase
2	-990.9917	1KZL	transferase
3	-906.5003	1C0A	ligase/RNA
4	-889.1661	1KGQ	transferase
5	-869.3531	1I95	ribosome
6	-860.2331	1JR4	transferase
7	-858.0005	1A2N	transferase
8	-832.0515	1NKK	hydrolase
9	-788.3545	1JIL	ligase
10	-757.2852	1EJB	transferase
11	-697.9477	1DMT	hydrolase
12	-645.0269	1PAU	complex (protease/inhibitor)
13	-633.1260	1F74	lyase
14	-628.9678	1KYU	endocytosis/exocytosis
15	-616.4458	1NRS	serine proteinase/receptor
16	-608.4169	9LYZ	hydrolase (o-glycosyl)
17	-600.2775	1EIO	lipid-binding protein
18	-593.7082	1F7B	lyase
19	-585.7663	1LMW	complex (serine protease/inhibitor)
20	-584.0059	1R1R	oxidoreductase
21	-580.1563	1IL2	ligase/RNA
22	-573.0481	1BLL	hydrolase(alpha-aminoacylpeptide)
23	-572.6763	1E1F	glycoside hydrolase
24	-540.1965	1LKL	complex (tyrosine kinase/peptide)
25	<b>-524.2817</b>	<b>1UK4</b>	<b>hydrolase</b>
26	-518.3528	1LCB	transferase (methyltransferase)
27	-506.8123	1PGN	oxidoreductase (choh(d)-nadp+(a))
28	-493.5477	1I5Q	hydrolase
29	-486.8954	1KYD	endocytosis/exocytosis
30	-481.9659	1NRR	serine proteinase/receptor

FIG.81

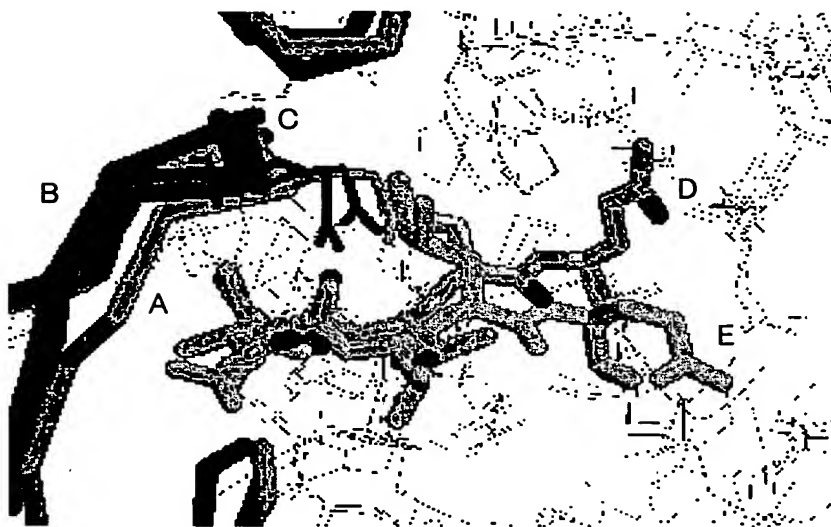


FIG.82





FIG.83

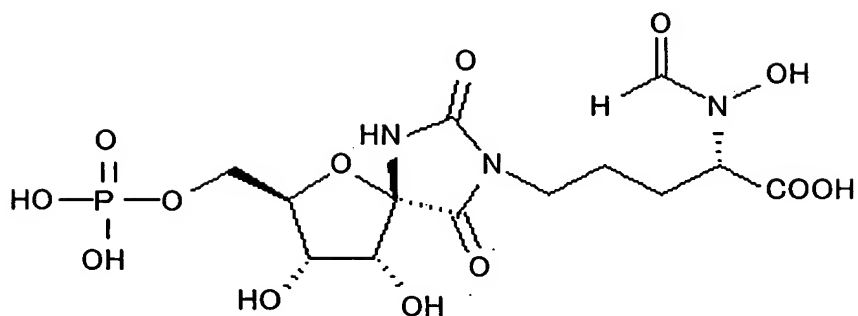


FIG.84

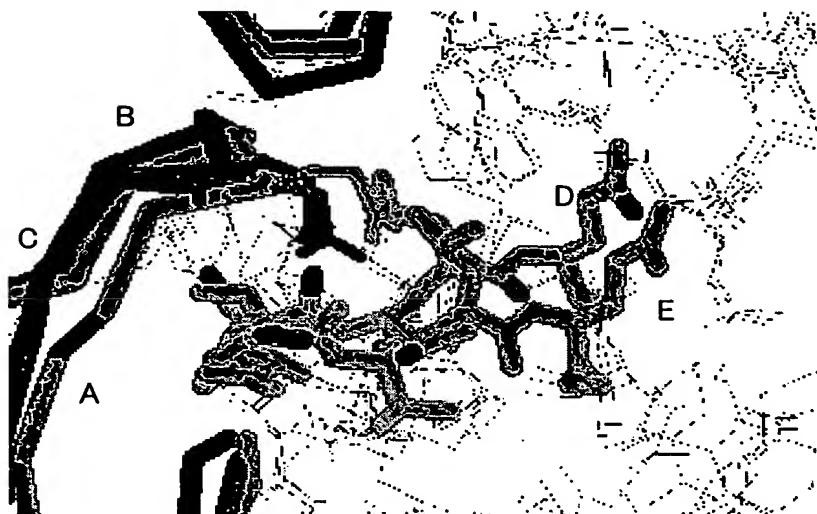
ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
CYS145 N	O.co2	100	2.70
GLU 166 N	O.2	100	2.70
THR190 N	O.3	100	2.70

Title: LIGAND SEARCHING DEVICE,  
LIGAND SEARCHING METHOD,  
PROGRAM, AND RECORDING  
MEDIUM

Inventor(s): Hideaki UMEYAMA et al.  
Appl. No.: Unassigned

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FIG.85



## FIG.86

RANKING	ENERGY	PDB code	REMARKS
1	-1263.8870	1EAD	dihydrolipoamide acetyltransferase
2	-1260.8689	1F6M	oxidoreductase
3	-1147.1739	1JR4	transferase
4	-1141.9917	1QF5	ligase
5	-1104.9447	1JAY	structural genomics
6	-1019.3584	1KZL	transferase
7	-996.5865	1QF4	ligase
8	-988.6588	1JIJ	ligase
9	-981.8594	8ICO	complex (nucleotidyltransferase/dna)
10	-953.0986	1LO9	hydrolase
11	-949.1903	1JTU	transferase
12	-922.4795	1JKX	transferase
13	-918.4892	1JIL	ligase
14	-916.9950	1I95	ribosome
15	-908.4880	1AL6	lyase
16	-893.5862	1LKL	complex (tyrosine kinase/peptide)
17	-892.3713	1N37	deoxyribonucleic acid
18	-887.9721	1LCB	transferase (methyltransferase)
19	-866.9600	1O9F	protein binding
20	-826.4893	1LO7	hydrolase
21	-792.0254	4UAG	ligase
22	-776.9998	1EJB	transferase
23	-772.2400	1BFZ	n-terminal product peptide
24	-769.6844	1F9E	apoptosis
25	-762.5275	1TLP	hydrolase (metalloproteinase)
26	-759.8312	1QIN	lyase
27	-758.2140	1KO6	transferase
28	-757.5526	1C0A	ligase/RNA
29	-755.7987	1QD1	transferase
30	-755.1049	1LO8	hydrolase
49	-639.1858	1UK4	hydrolase

FIG.87

ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
THR25 OG1	N.am	100	3.80
CYS145 N	O.co2	100	2.70
MET165 CG	C.3	100	4.00
GLU166 N	O.2	100	2.70
THR190 N	O.3	100	2.70

FIG.88

RANKING	ENERGY	PDB code	REMARKS
1	-364.6548	1I95	ribosome
2	<b>-299.0166</b>	<b>1UK4</b>	<b>hydrolase</b>
3	-109.6867	1BXX	endocytosis/exocytosis
4	-93.0540	1KZL	transferase
5	-72.9399	1NKK	hydrolase
6	-10.7565	1F8H	endocytosis/exocytosis
7	-4.2756	1QTN	apoptosis
8	162.1557	1KGQ	transferase
9	163.2075	1O9F	protein binding
10	331.8725	1CGL	metalloprotease
11	370.5027	2BBQ	transferase(methyltransferase)
12	397.8488	4DMR	oxidoreductase
13	550.2598	1HPG	hydrolase (serine protease)
14	716.6561	1LOC	lectin
15	839.7398	1DMT	hydrolase
16	848.7090	1KAP	zinc metalloprotease
17	850.2630	1JG3	transferase
18	883.4400	1BC5	complex (methyltransferase/peptide)
19	905.9695	1FCH	signaling protein
20	913.9769	1CF8	catalytic antibody
21	1088.2428	1NWE	hydrolase
22	1089.3496	1KO6	transferase
23	1116.9042	1F74	lyase
24	1131.4783	1ING	hydrolase (o-glycosyl)
25	1132.3648	1I31	endocytosis/exocytosis
26	1148.9063	1IAU	hydrolase
27	1156.0335	1B48	transferase
28	1160.3512	1PTT	complex (hydrolase/peptide)
29	1176.7814	1MC5	oxidoreductase
30	1197.3565	1F9E	apoptosis

FIG.89



FIG.90

ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
CYS145 N	ACCEPTOR	100	2.70
MET165 CG	CARBON	100	4.00
GLU166 N	ACCEPTOR	100	2.70
THR190 N	ACCEPTOR	100	2.70

Title: LIGAND SEARCHING DEVICE,  
LIGAND SEARCHING METHOD,  
PROGRAM, AND RECORDING  
MEDIUM

Inventor(s): Hideaki UMEYAMA et al.  
Appl. No.: Unassigned

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## FIG.91

RANKING	ENERGY	PDB code	REMARKS
1	-2095.8588	1JJQ	hormone/growth factor
2	-2011.3626	2BVW	hydrolase
3	-1670.8384	1DOG	hydrolase
4	-1336.7960	1LWJ	transferase
5	-1320.0704	1KEU	lyase
6	-1230.0604	1GAH	hydrolase
7	-1214.9459	1I7E	signaling protein
8	-1195.8653	1C39	signaling protein
9	-1191.3777	1BB5	hydrolase
10	-1189.0253	2FHI	nucleotide-binding protein
11	-1147.9761	1GO6	glycopeptide antibiotics
12	-1103.6272	1M4D	transferase
13	-1095.3050	1QHC	hydrolase
14	-1088.7299	1M2N	gene regulation
15	-1078.3684	1QGL	lectin (agglutinin)
16	-1056.4078	4ENG	glycosyl hydrolase
17	-1033.0227	1LON	ligase
18	-1031.2555	1MWL	ribonucleic acid
19	-1027.4239	1QPK	hydrolase
20	-1014.9817	1UDB	isomerase
21	-1005.1689	1GQC	transferase
22	-976.9293	1H6H	px domain
23	-975.2827	1LSP	hydrolase (o-glycosyl)
24	-973.5218	1FF1	signaling protein
25	-963.4098	3UAG	ligase
26	-937.2165	1IBG	immunoglobulin
27	-933.6818	1DRV	oxidoreductase
28	-918.6947	2MBR	oxidoreductase
29	-917.1703	1NAB	deoxyribonucleic acid
30	-897.3026	1SLY	glycosyltransferase
774	331.9928	1UK4	hydrolase

FIG.92

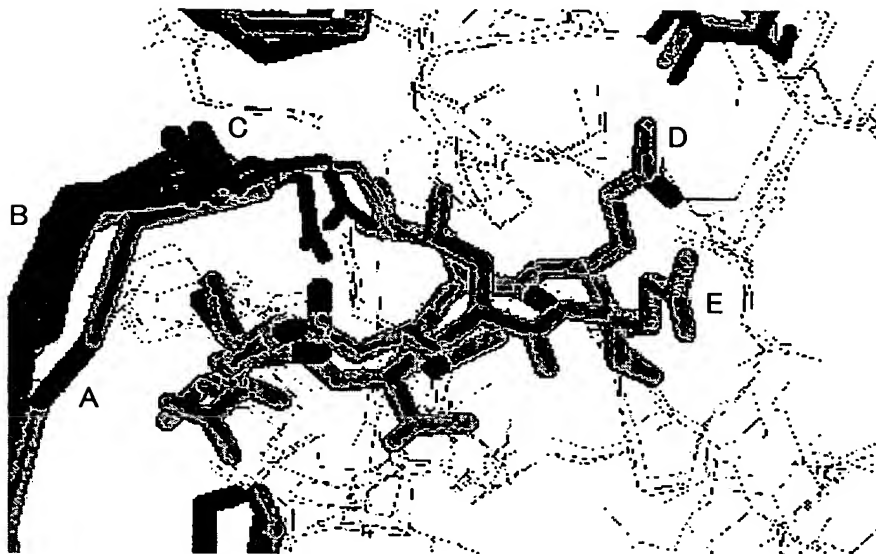


FIG.93

ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
CYS145 N	O.co2	100	2.70
MET165 CG	C.3	100	4.00
GLU166 N	O.2	100	2.70
THR190 N	O.3	100	2.70

## FIG.94

RANKING	ENERGY	PDB code	REMARKS
1	-1047.3743	1KZL	transferase
2	-860.437	1J71	hydrolase
3	-844.8737	3UAG	ligase
4	-837.6255	1LKL	complex (tyrosine kinase/peptide)
5	-829.8176	1QF4	ligase
6	-732.2087	1A2N	transferase
7	-721.6213	1G1F	hydrolase, signaling protein
8	-698.5922	1F7B	lyase
9	-689.1472	1BFZ	n-terminal product peptide
10	-646.7943	148L	hydrolase(o-glycosyl)
11	-634.4654	1CGL	metalloprotease
12	-629.1673	1JIL	ligase
13	-616.8733	1FF1	signaling protein
14	-611.1171	1F9E	apoptosis
15	-567.0738	1R1R	oxidoreductase
16	-554.5321	1I95	ribosome
17	-547.2494	1FQX	hydrolase
18	-536.7069	1HCT	complex (signal transduction/peptide)
19	-531.1014	1SIA	mucin motif
20	-508.9899	1JIJ	ligase
21	-507.9655	1LSP	hydrolase (o-glycosyl)
22	-497.6341	1F8H	endocytosis/exocytosis
23	-492.3974	1F74	lyase
24	-443.232	1QH5	hydrolase
25	-427.5925	1JII	ligase
26	-417.4991	1JQY	toxin
27	-416.9956	2KCE	methyltransferase
28	-396.7898	1EJB	transferase
29	-387.6441	1MMJ	hydrolase
30	-358.2162	1SLY	glycosyltransferase
39	-245.9500	1UK4	hydrolase



FIG.95

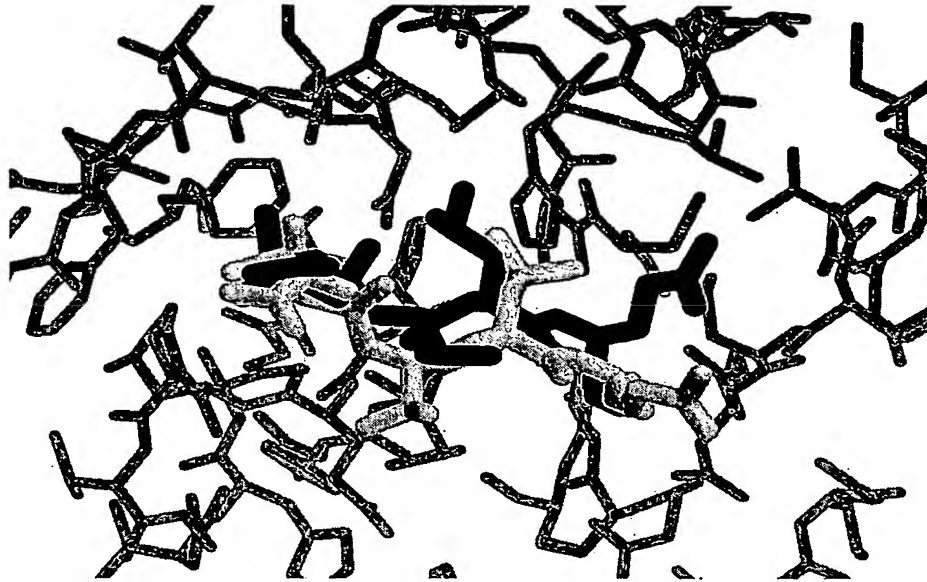


FIG.96

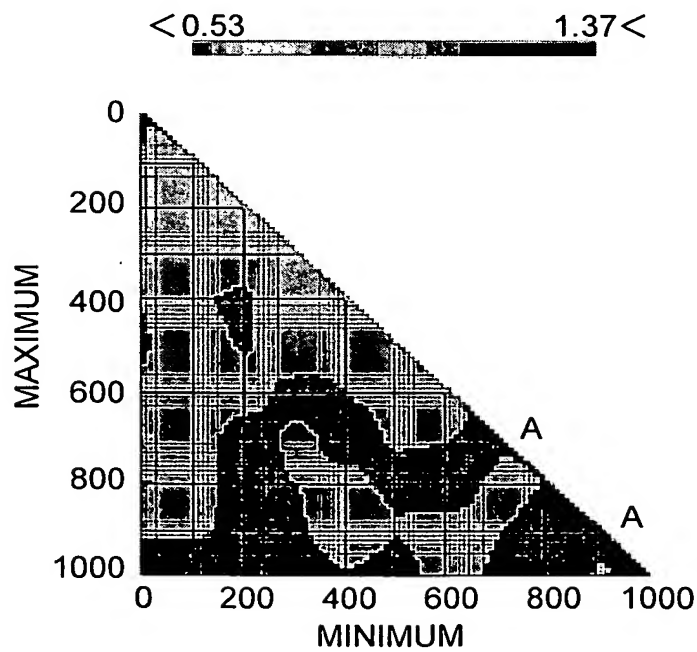


FIG.97

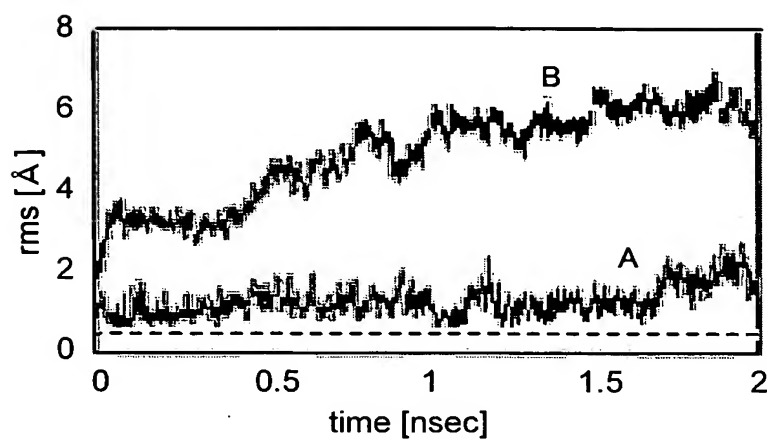


FIG.98

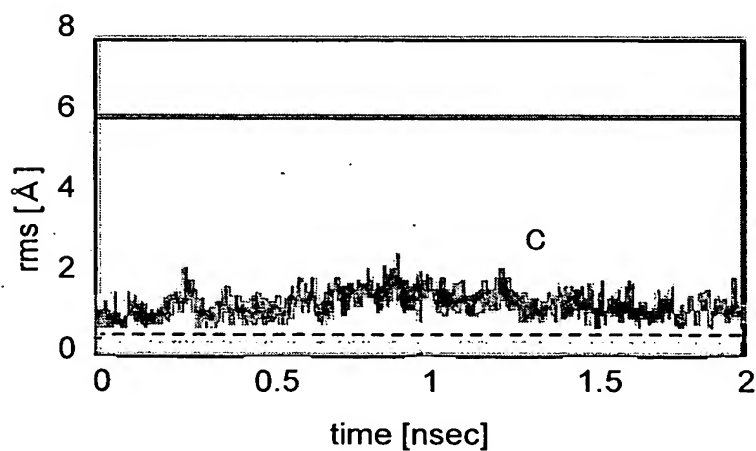


FIG.99

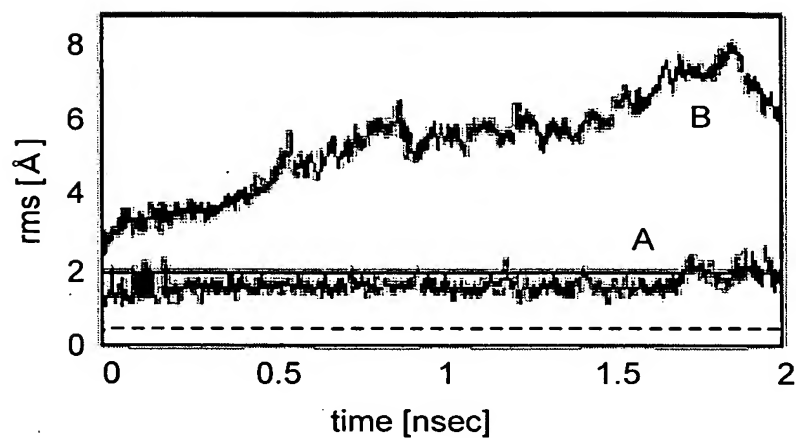


FIG.100

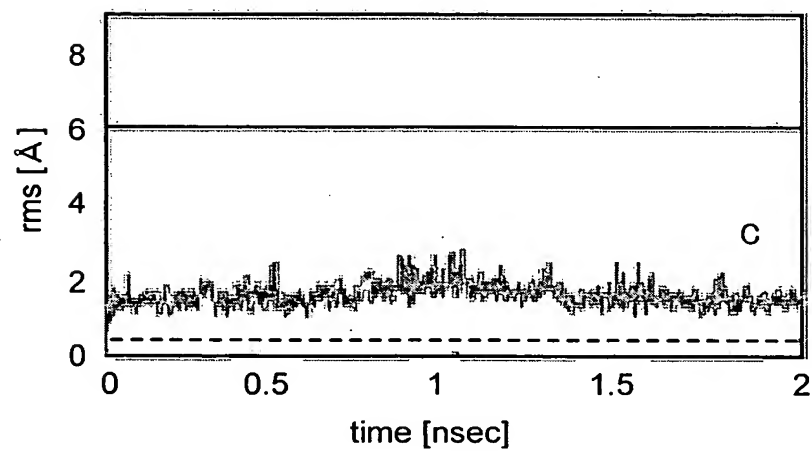


FIG.101

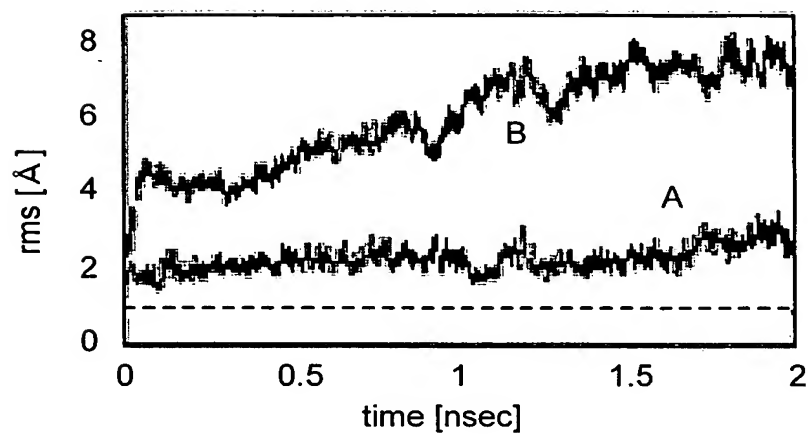


FIG.102

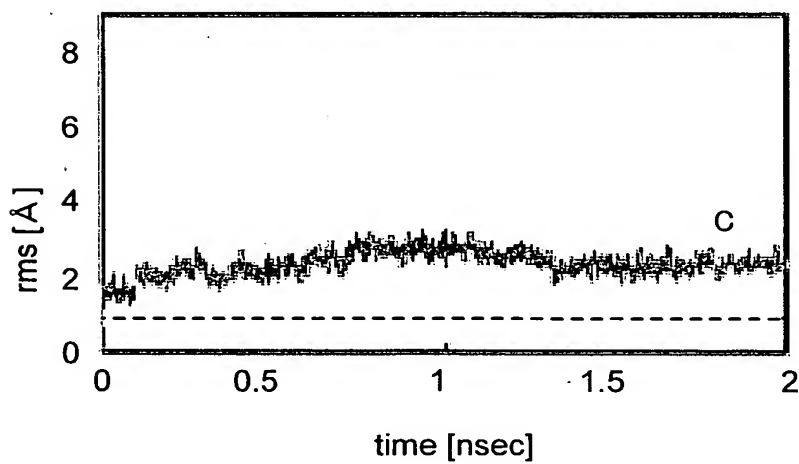


FIG.103

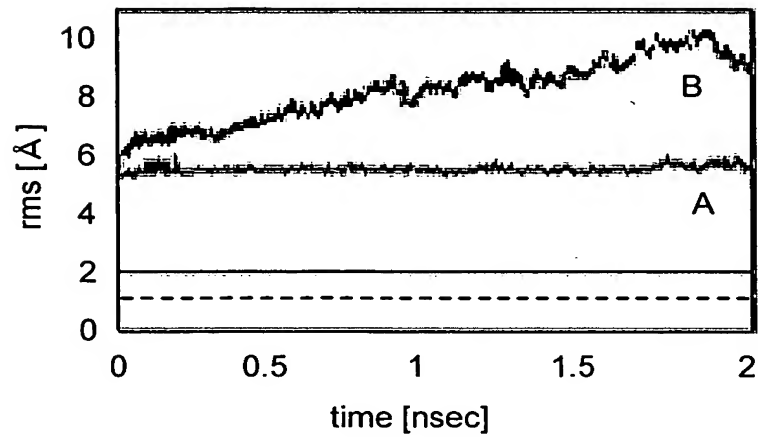


FIG.104

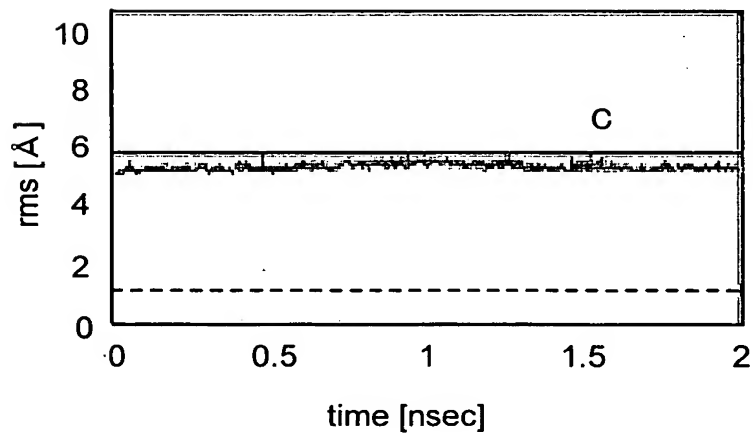


FIG.105

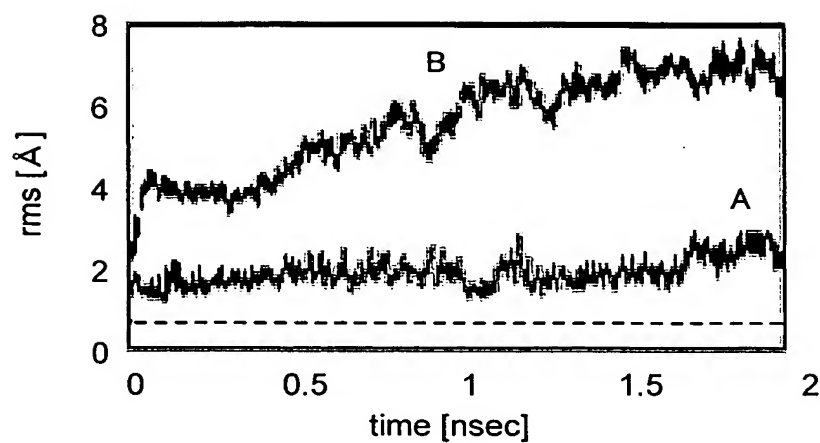


FIG.106

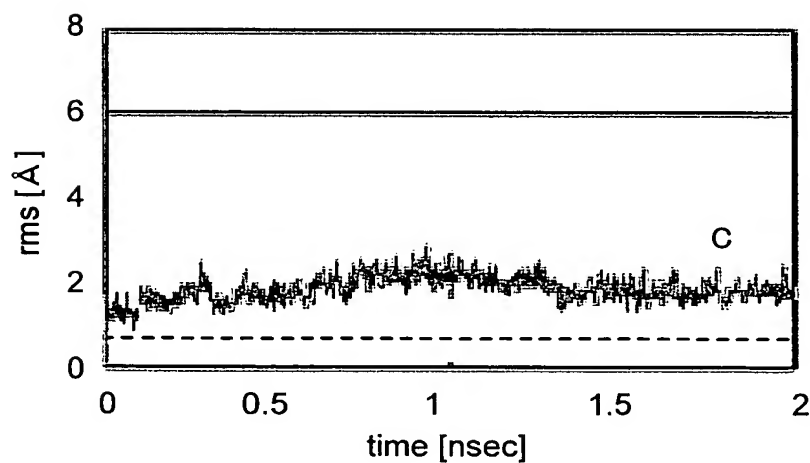


FIG.107

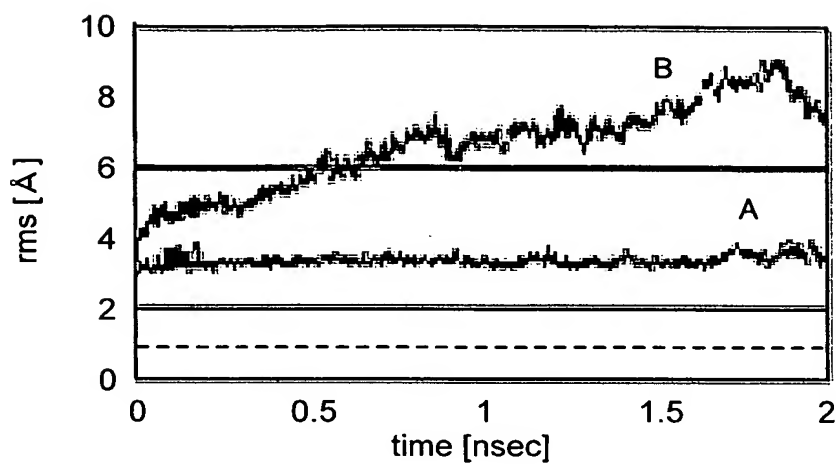


FIG.108

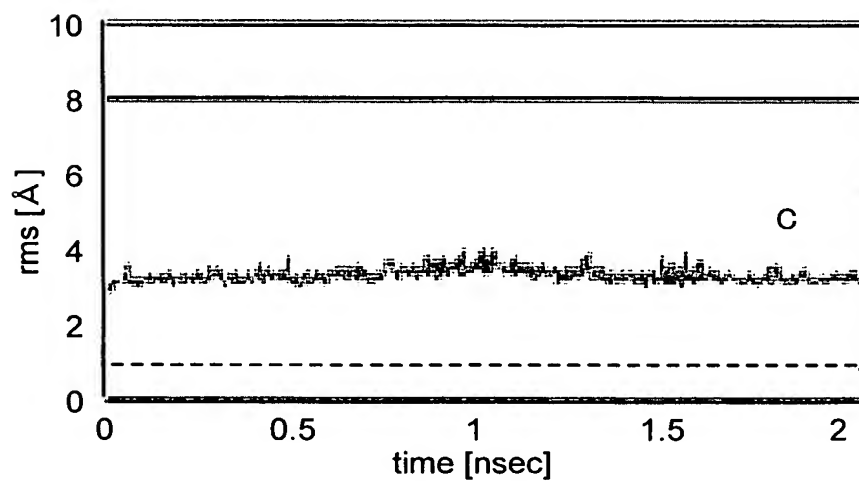


FIG.109

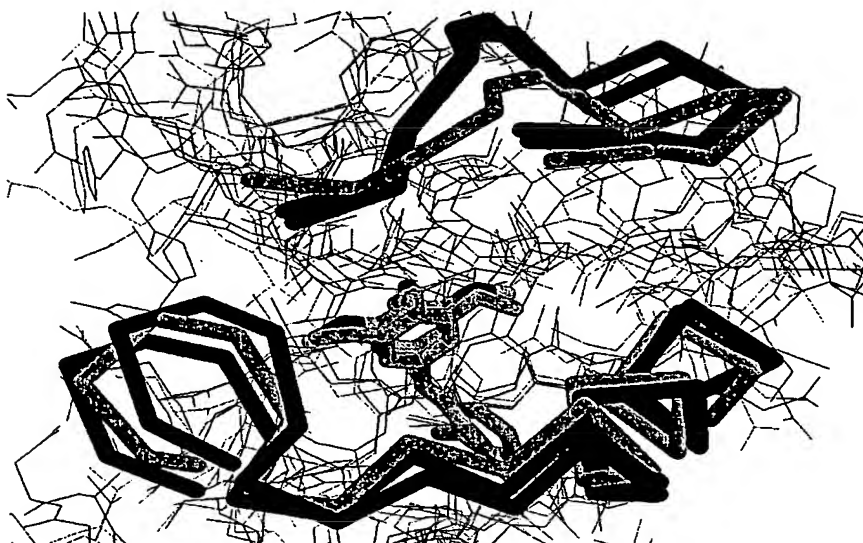


FIG.110

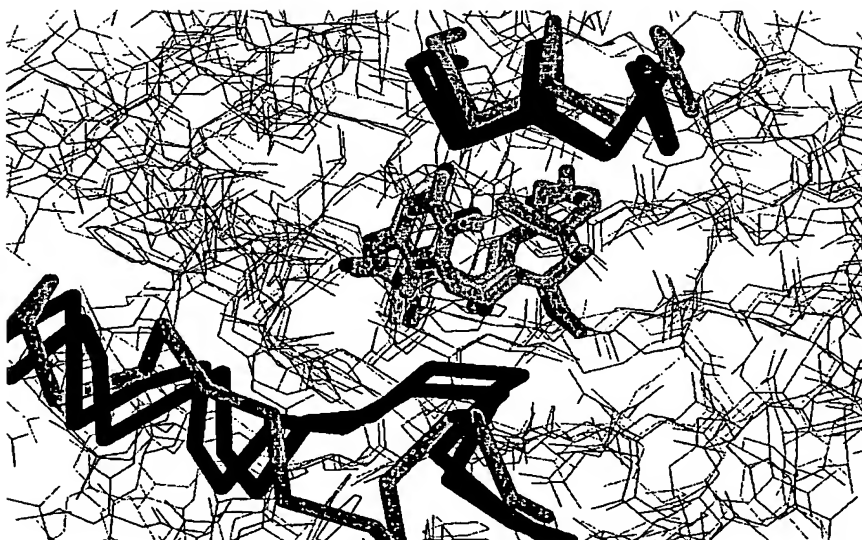




FIG.111

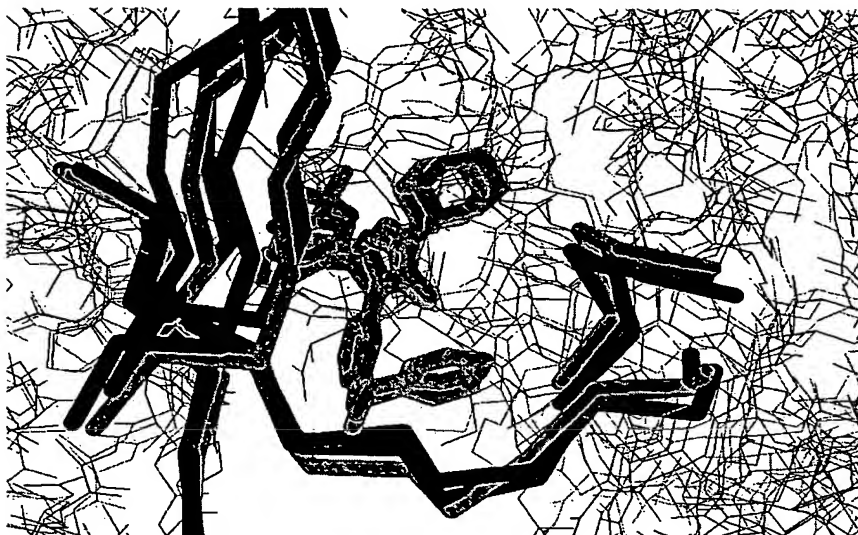


FIG.112

ATOM OF ACTIVE SITE	ATOM TYPE OF LIGAND	INTENSITY OF INTERACTION	DISTANCE OF INTERACTION [Å]
LUE4 O	N.pl3	100	2.87
ASP26 OD1	N.ar	300	3.00
ASP26 OD2	N.pl3	300	3.00

FIG.113



FIG.114

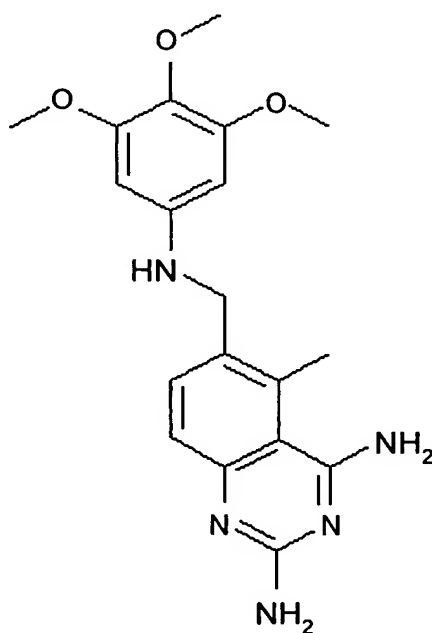


FIG.115

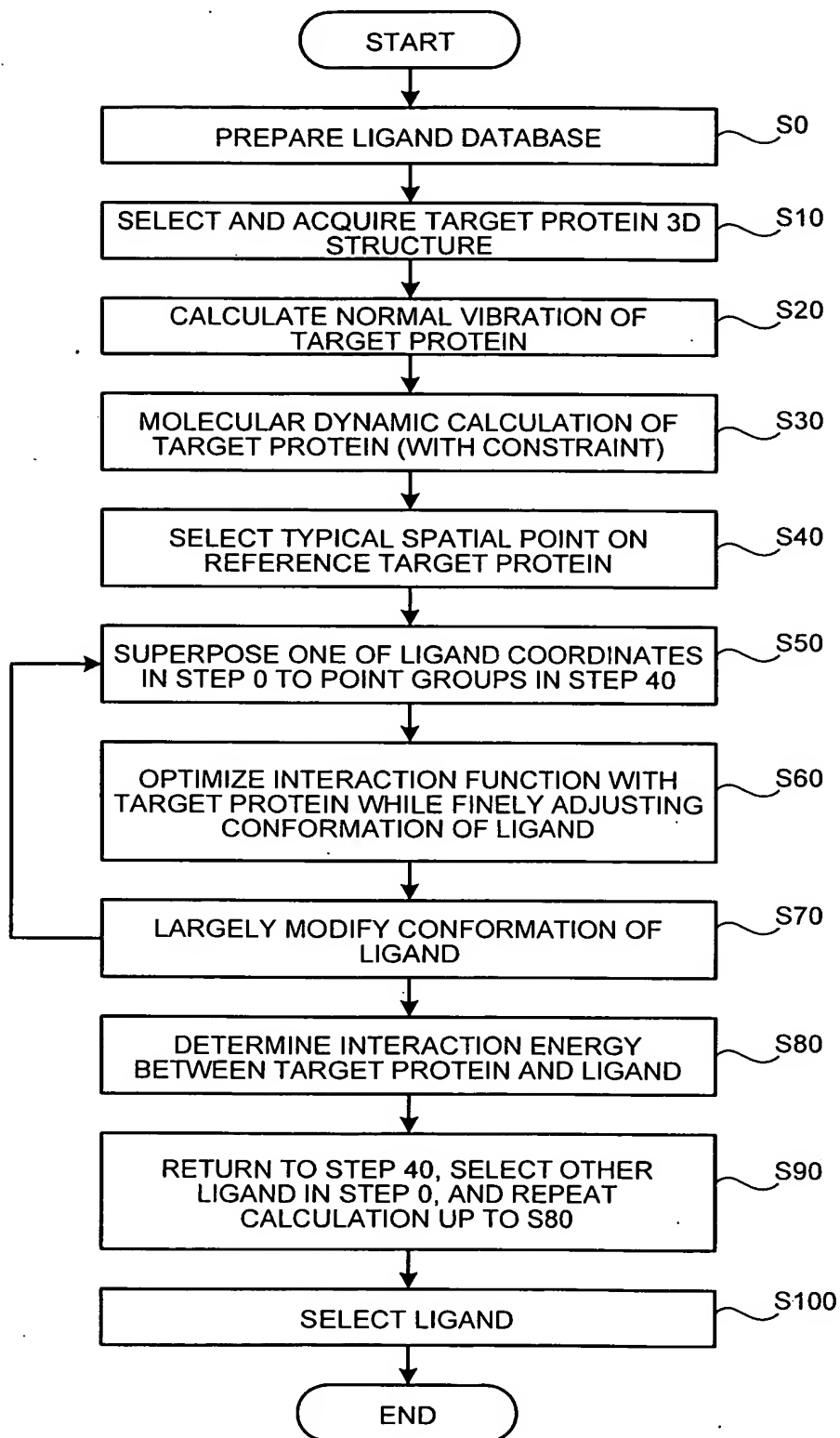


FIG. 116

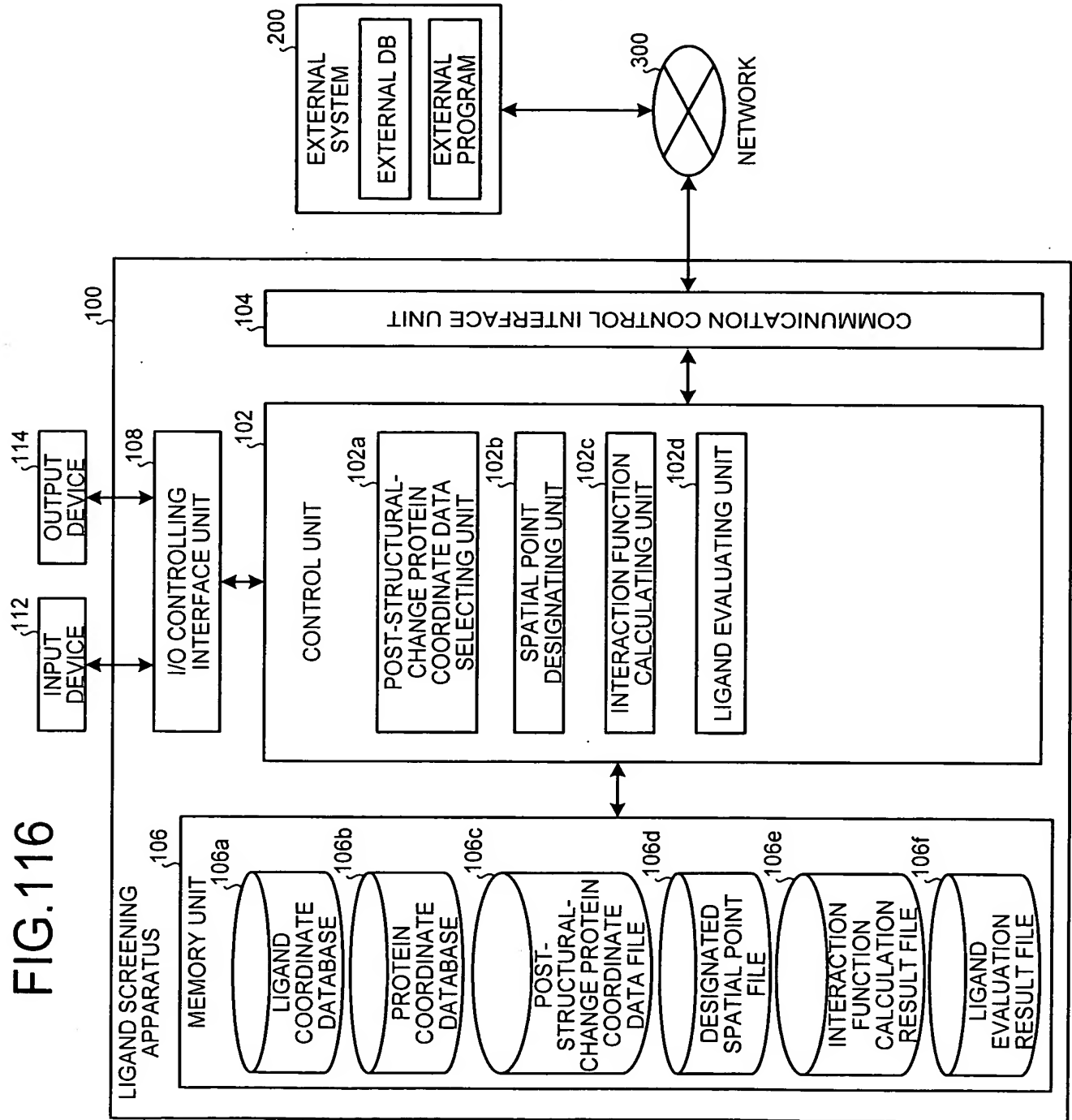


FIG.117

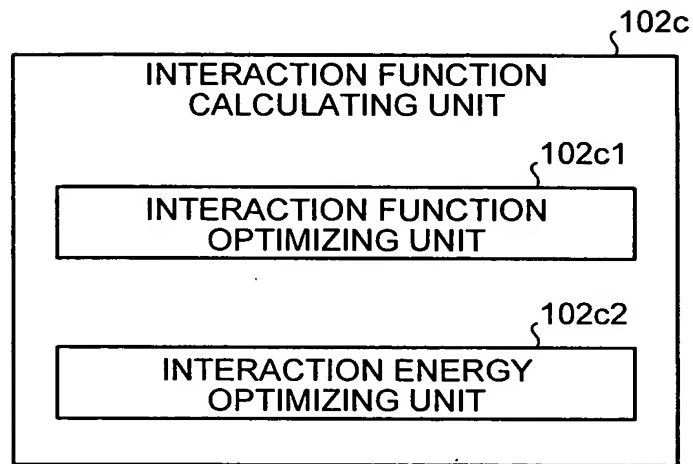
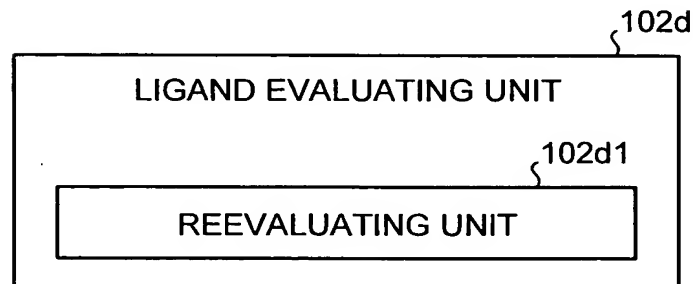


FIG.118



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